ACD/ChemSketch

Version 4.5 for Microsoft Windows

User's Guide

Drawing Chemical Structures and Graphical Images

Advanced Chemistry Development Inc.

Copyright © 1994-2000 Advanced Chemistry Development Inc. All rights reserved.

ACD/Labs is a trademark of Advanced Chemistry Development Inc.

Microsoft is a registered trademark and Windows is a trademark of Microsoft Corporation.

IBM is a registered trademark of International Business Machines Corporation.

All the other trademarks mentioned within this Manual are the property of their respective owners.

All trademarks are acknowledged.

Information in this document is subject to change without notice and is provided "as is" with no warranty. Advanced Chemistry Development Inc. makes no warranty of any kind with regard to this material, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. Advanced Chemistry Development Inc. shall not be liable for errors contained herein or for any direct, indirect, special, incidental or consequential damages in connection with the use of this material.

Table of Contents

1. Introduction 1

1.1 What is ACD/ChemSketch 1
1.2 Additional Modules 1
1.3 What's New in 4.5 2
1.4 About this Guide 3
1.5 Useful Definitions 3
1.6 Demo Versions 4
1.7 Freeware Version 4
1.8 For More Information… 4
1.8.1 How to Get Hold of Us 5

2. Basics of ACD/ChemSketch 6

2.1 Objectives 6
2.2 Starting ACD/ChemSketch 6
2.3 Structure and Draw Mode 7
2.3.1 Structure Mode Screen 7
2.3.2 Draw Mode Screen 8

3. Drawing Simple Structures 10

3.1 Objectives 10
3.2 Drawing Atoms, Bonds and Labels 10
3.2.1 Using the Draw Normal Tool 10
3.2.2 Using the Draw Continuous Tool 11
3.2.3 Using Mouse Drag 12
3.2.4 "Cleaning" the Structure 12
3.2.5 Using the Stereo, Coordinating and Undefined Bond Tools 12
3.2.6 Editing Atom Labels 13
3.2.7 Using the Draw Chains Tool 14
3.3 Flipping Structures 15
3.4 Selecting, Rotating, and 3D Rotating 15
3.5 Clearing the Screen 16

4. Drawing More Complex Structures 17

4.1 Objectives 17
4.2 Using the Table of Radicals 17
4.3 Using Ring Structures 18
4.4 Deleting Atoms and Fragments 18
4.4.1 Deleting Atoms Individually 19
4.4.2 Deleting All Atoms Simultaneously 19
4.5 Replacing Atoms 19
4.6 Setting Double and Triple Bonds 20
4.7 Setting Charges and Defining Anions and Cations 21
4.8 Changing Atom Properties 23

5. Advanced Structures and Reaction Schemes 24

5.1 Objectives 24
5.2 2D Optimization 24
5.2.1 Creating the Structure of Cyclic Alkanes 24
5.2.2 Creating the Structure of a Cyclic Peptide 25
5.3 3D Optimization 26
5.3.1 Creating Structure of Bicyclo[2.2.2]octane 27
5.3.2 Creating the Structure of Triptycene 28
5.3.3 Creating the Structure of Cubane 29
5.3.4 Creating the Structure of Dodecahedrane ([5]Fullerene-C_{20}) 30
5.4 Drawing a Reaction Scheme 32

6. Advanced Drawing: Templates 34

6.1 Objectives 34
6.2 Overview 34
6.3 Instant Template Tool 35
6.3.1 Creating the Structure of a Cyclic Oligomer 35
6.4 Table of Radicals in Structure Drawing 37
6.4.1 Creating the Structure of Fluorescamine 37
6.5 Templates from the Template Window 38
6.5.1 Creating the Fragment of a DNA Molecule 38
6.5.1.1 Drawing the chain of deoxyriboso-5-phosphate fragments 39
6.5.1.2 Adding the bases 40
6.6 Drawing Complex Biomolecules 40
6.6.1 Creating the Structure of β-Maltose 40
6.7 Defining a User Template 42
6.7.1 The Template.cfg File 43
6.7.2 Available Templates 43

7. Creating Special Graphical Objects 44

7.1 Objectives 44
7.2 Drawing the Energy of Reaction Diagram 44
7.2.1 Drawing a Curve 44
7.2.2 Drawing the X and Y axes 45
7.3 Drawing Different Kinds of Orbitals 46
7.4 Drawing Vacuum Distillation Apparatus 49
7.5 Drawing a Two-chain DNA Strand 51
7.6 Drawing Lipids and Micelles 55
7.6.1 Drawing the lipid 55
7.7 Creating a Poster 57

8. Calculating Macroscopic Properties 59

8.1 Overview 59
8.2 Calculating Macroscopic Properties 59
8.2.1 Menu Command 59
8.2.2 Automatic Display on Status Line 60
8.3 Algorithms for Calculating Macroscopic Properties 61
8.3.1 Molar Volume, MV 61
8.3.2 Molar Refractivity, MR 62
8.3.3 Parachor, P_r 62
8.3.4 Density, d 62
8.3.5 Refractive Index, n 62

8.3.6 Surface Tension, γ *62*
8.3.7 Dielectric Constant, ε (Permittivity) *63*
8.3.8 Polarizability *63*
8.4 Correlation Statistics with Experimental Data 63
8.4.1 Distribution of Molar Refractivity Prediction Error *63*
8.4.2 Distribution of Molar Volume Prediction Error *64*
8.4.3 Distribution of the Parachor Prediction Error *64*
8.4.4 Distribution of the Refractive Index Prediction Error *65*
8.4.5 Distribution of the Density Prediction Error *65*
8.4.6 Distribution of the Surface Tension Prediction Error *66*
8.4.7 Distribution of the Dielectric Constant (Permittivity) Estimation Error *66*

9. Special Function Keys 67

9.1 Tautomers 67
9.2 Dictionary 68

10. Goodies 69

10.1 What are “Goodies”? 69
10.2 Where can I get them? 69
10.3 Goodies 69

1. Introduction

1.1 What is ACD/ChemSketch

ACD/ChemSketch is a chemical drawing software package from Advanced Chemistry Development, Inc. designed to be used alone or integrated with other applications. ChemSketch is used to draw chemical structures, reactions and schematic diagrams. It can also be used to design chemistry-related reports and presentations.

ACD/ChemSketch has the following major capabilities:

- **Structure Mode** for drawing chemical structures and calculating their properties.
- **Draw Mode** for text and graphics processing.
- **Molecular Properties** calculations for automatic estimation of:
  - molecular weight;
  - percentage composition;
  - molar refractivity;
  - molar volume;
  - parachor;
  - index of refraction;
  - surface tension;
  - density;
  - dielectric constant; and
  - polarizability.

ACD/ChemSketch can stand alone as a drawing package or act as the “front end” to other ACD software such as the NMR Predictor engines.

1.2 Additional Modules

There are additional ACD software items which are accessible through the ChemSketch interface, as single-click buttons. These items, which are increasing in number with each upgrade, are available as additional options and should be considered as separate items. All of them have separate guides. Please contact us or consult our Web site for more details on pricing and availability.

- **ChemBasic** - the special programming language that enables the user to customize ACD software (can be downloaded from http://www.acdlabs.com). As of Spring 2000, ChemBasic version 1.3 freeware is available from our web site. Please see Chapter 10, “Goodies”, for some examples of how ChemBasic can be used with ChemSketch.
- **ACD/I-Lab** - the Internet-based service that allows you to get instant access to chemical databases and property predictions programs. An account on the Interactive Lab can be set up from http://www.acdlabs.com/ilab . As of Spring 2000, a 2-week demo period can be arranged for the I-Lab. ChemSketch 4.0 and upwards can access the I-Lab automatically, if run on a PC with Internet connection.

- **ACD/Tautomers** - checks and generates the most reasonable tautomeric forms of organic structures (included in both freeware and commercial versions of ChemSketch);
- **ACD/Dictionary –** looks up the molecular structure for common drug names. ACD/Dictionary contains over 48,000 systematic and non-systematic names of the most frequently used chemicals and biologicals. The entries cover more than 200 therapeutic areas, and the inhibitors of more than 500 different enzymes are also available (included in commercial version only).

The following buttons represent functionality that must be purchased in addition to ACD/ChemSketch:

- **ACD/pKa Calculator** - calculates accurate acid-base ionization constants at 25 degrees Celsius and zero ionic strength for a structure as drawn in the ChemSketch window;
- **ACD/LogP Calculator -** calculates octanol-water partition coefficients (log P values) for neutral molecule as drawn in the ChemSketch window;
- **ACD/Boiling Point and Vaporization** - calculates accurate boiling points at any pressure from 0.001 mm Hg to 10 atm, in most cases to ±10 degrees or better, for a structure as drawn in the ChemSketch window;
- **ACD/Solubility** - calculates the solubility of the sketched-in structure as a function of pH;
- **ACD/Sigma** - displays the Hammett-type or related parameters for different substituent groups as drawn in the ChemSketch window;
- **ACD/Name to Structure** – generates a molecular structure for almost any chemical name typed in. ACD/Name to Structure treats most names of general organic compounds and many natural products derivatives according to IUPAC recommendations on Organic, Biochemical and Inorganic Nomenclature.

1.3 What's New in 4.5

If you are new to this software, we recommend that you work through the examples described in the following chapters. If, however, you have purchased (or are thinking of purchasing) this software as an upgrade, you are likely already familiar with the basic features of ChemSketch. In this section we list only the newest features.

- **Reaction Plus** and **Reaction Arrows** tools are now available directly in the Structure mode. You do not have to switch to the Draw mode for drawing these objects.
- The new **Reaction** tab in the **Preferences** dialog box (**Options** menu) allows you to choose among various options for Reaction Plus and Reaction Arrows.
- Graphical objects (those created in the Draw mode) can now be selected and moved in the Structure mode as well. This facilitates the drawing of complex reports. To enable this feature, make sure that the **Select Graphics** check box is selected in the **Structure** tab of the **Preferences** dialog box (**Options** menu).
- Stereo configuration can be controlled when the **Clean** and **Flip** tools are applied. See the bottom part of the **Structure** tab in the **Preferences** dialog box (**Options** menu).
- New structure file formats can be imported: ChemDraw CDX (*.cdx) files and REACCS RXN (*.rxn) files. The RXN format is also a newly-supported Export format.
- A new additional module can be purchased to be integrated into the ChemSketch Window - ACD/Name to Structure (refer to section 1.2 for more details).

- The ACD/I-Lab add-on allows you to access our prediction modules and various chemical databases via Internet. Just sign up for an account on the Interactive Lab at http://www.acdlabs.com/ilab . (As of Spring 2000, a 2-week demo period can be arranged for the I-Lab.) The I-Lab can be accessed automatically, if run on a PC with Internet connection.

1.4 About this Guide

To start using ACD/ChemSketch in its full power you don't have to read a manual, it is so intuitive and simple to use. That's why this guide doesn't provide comprehensive descriptions of all the options available in the program; rather, it just gets you started. After reviewing these exercises, you will be able to use ACD/ChemSketch yourself, without any further assistance and with maximum speed and efficiency.

You will be able to view nearly every section of this manual in **animated form** in the LotusCam®-based **movies**, downloadable from our Web site (www.acdlabs.com). (These movies are also present on our demo CD as well as the installation CD.)

This User's Guide is provided in electronic form, readable with a commonly-available word processing program. If you cannot locate an index topic you need, please do a text string-search in the word processing program for the relevant word or phrase, or related words.

The screen-shots shown throughout this tutorial have been taken with a relatively small window size. The default display is a window which fills the screen. Click once on the Minimize button (upper right-hand corner of window display) to get a smaller working area; click on the Maximize button to return to full-screen display.

The screen-shots have been taken with the next-to-last version of the software. We have made every effort to match what you will see in ACD/ChemSketch with what the tutorial shows, but there may be slight discrepancies.

This Guide assumes you have basic familiarity with mouse and file manipulation in Microsoft Windows.

1.5 Useful Definitions

In this tutorial the following terms are used to describe various actions:

Point means move the mouse pointer to an item.

Click or **left-click** means move the mouse pointer to an item, and press the left mouse button.

Right-click means move the mouse pointer to an item, and press the right mouse button.

Double-click means move the mouse pointer to an item, and quickly press the left mouse button twice.

Drag means press and hold down the left mouse button while you move the mouse.

Note In Windows the default mouse button side is on the left. You can change the default side to the right by summoning the **Mouse** dialog box from the **Windows Control Panel**. (This also permits you to change the speed and motion attributes of the mouse.)

1.6 Demo Versions

When the demo version is first loaded to run, you will see a message displayed that informs you this is ACD Demonstration software. You may also see this message displayed from time to time throughout the normal course of using the demo software.

Demo versions of ACD/Labs programs have **some command restrictions** such as Save, Copy, Cut, Paste and Print features. If you try to carry out a restricted operation from a demo version, a dialog box will appear which informs you that it is not permitted.

If you would like to know more about a specific restriction in the full version of the program, please contact us. Nevertheless, most of the exercises and examples in this guide are designed so that you can execute them with the demo version of this ACD/Labs program as well.

1.7 Freeware Version

From April 1999 onward, Advanced Chemistry Development has been making ChemSketch 4.0 available as freeware, through the "Free Stuff" link at our web site. Please be advised that the freeware version:

(a) does not come with ACD/Dictionary;
(b) does not have the latest enhancements for version 4.5 (see section 1.4, "What's New");
(c) does not include ACD Add-ins for ISIS/Base or ISIS/Draw; and
(d) does not entitle you to technical support. (However, there is a newsgroup at news://news.acdlabs.com/acd.public.chemsketch where users can post their questions or share tips.)

The freeware ChemSketch:

(a) does come with ACD/Tautomers and ACD/3D Viewer;
(b) does include a 15-second sequence listing our other products when it is first started up. Once the Cancel button becomes active, click it to remove this screen; and
(c) should be installed to its own separate folder. This folder can contain other ACD freeware concurrently available, such as ACD/SpecViewer, ACD/CNMRView, ACD/HNMRView, etc. but should not contain any purchased ACD software.

1.8 For More Information…

To see the latest in ACD software and services, please visit our web-site at

http://www.acdlabs.com

Our web-site is being accessed at the rate of tens of thousands of "hits" per day. There's a reason for this: much is offered through our web-site. As of Spring 2000, we offer free ChemSketch 4.0, a free ISIS 3D Add-in, free ChemDraw extensions and a free 2-week demo key for "Interactive Lab" sessions where you can run test calculations using Java applets without purchasing software. There are Lotus Cam-based movies which show the operation of many of our software packages available for download.

We are constantly updating the information on our web-site. The web-site will tell you at which scientific conferences you can visit the ACD booth. You can browse the Frequently Asked Questions page or drop in and "chat" on our newsgroup, which can also be reached via our web page.

If you would like to stay informed of the latest developments in chemical naming software products at ACD, please be sure to sign up for e-mail broadcasts at our web site page:

http://www.acdlabs.com/feedback/mailing.html

If you would like to partake of the ChemSketch newsgroup, please access:

news://news.acdlabs.com/acd.public.chemsketch

1.8.1 How to Get Hold of Us

We are accessible through our web-site, phone, fax and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability and general issues should be directed to

info@acdlabs.com.

Technical and scientific support issues should be addressed to

support@acdlabs.com.

Please tell us the name of the software owner, the version number and release date of the product you are contacting us about. (This information is available by selecting Help/About.) If applicable, please tell us the name of the distributor from whom you purchased the software.

2. Basics of ACD/ChemSketch

2.1 Objectives

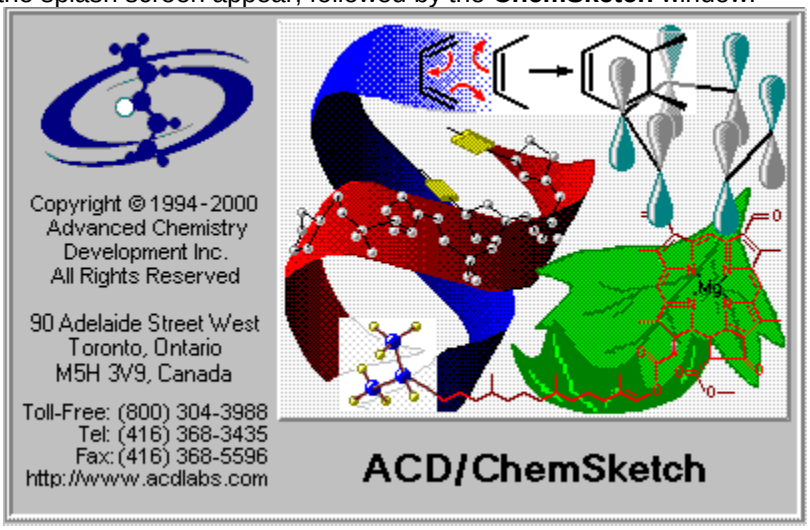
This Chapter will familiarize you with

- how to start the program;
- basics of the ChemSketch interface, namely, the Structure and Draw modes.

2.2 Starting ACD/ChemSketch

Once ACD/ChemSketch has been installed on your computer, follow these basic steps to start it:

1. Start Windows.
2. Double click on the ACD/ChemSketch icon to start ACD/ChemSketch.
   OR choose the ACD/ChemSketch icon from the Start/Run menu in the Windows 95 or NT Taskbar
   OR double click on the program file “chemsk.exe” in the ACD folder.
3. You will see the splash screen appear, followed by the **ChemSketch** window:



4. If this is the freeware version, you will see a 15-second list of ACD products scroll by. Be patient and click Cancel when it becomes active.
5. Then you will see a Tip of the Day box, which you can close after reading.

2.3 Structure and Draw Mode

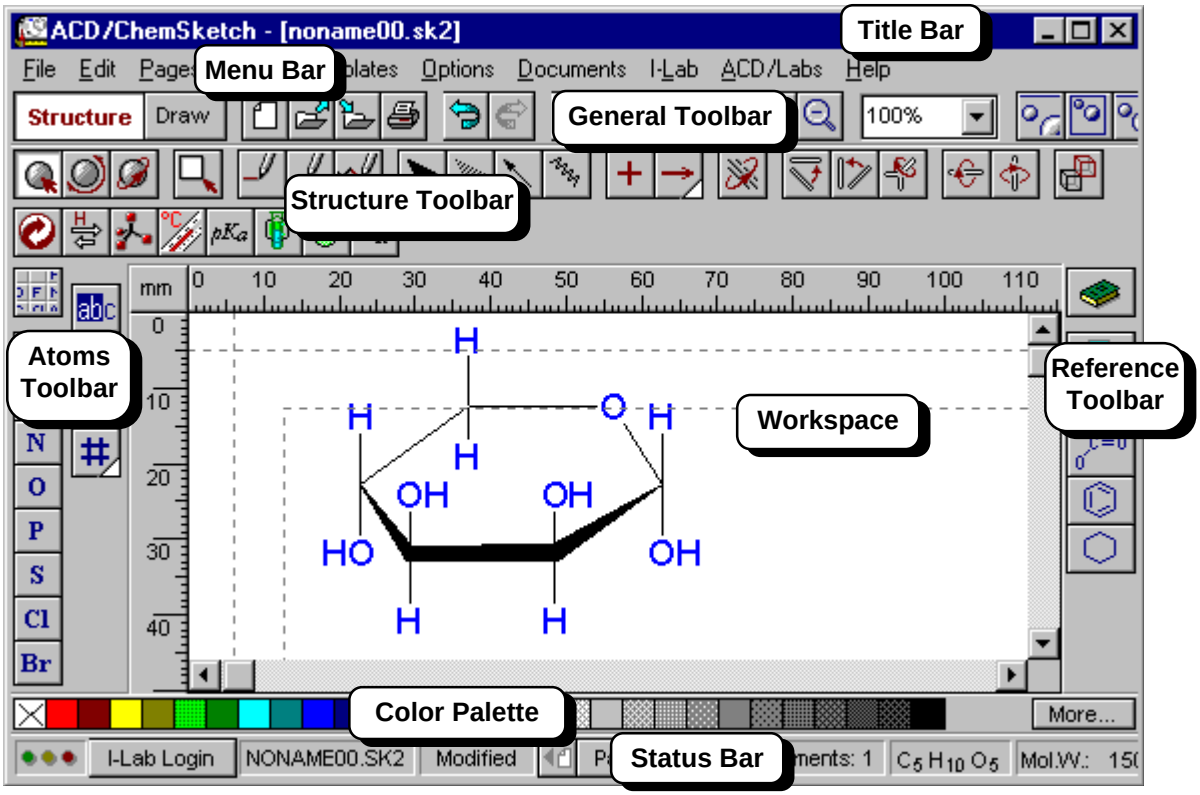
When ACD/ChemSketch starts up, you will find many menu commands and toolbar buttons dimmed (inactive). They will be enabled as soon as you draw a structure.

In the ChemSketch Window, there are two modes, **Structure** and **Draw.** You switch between them using the buttons in the upper left-hand corner:

In the Structure Mode you draw structures and reaction schemes while the Draw Mode presents you with the tools for entering text and drawing various graphical objects.

2.3.1 Structure Mode Screen

Below you can see the screen with the Structure Mode enabled. Please pay attention to the names and position of the toolbars, since we are going to use these terms throughout the whole Guide.



Title bar shows the name of the program and the name of the currently open file. The default file name is NONAMExx.SK2, where 'xx' is a counter.

Menu bar contains a series of words. Each word links to a list ('menu') of related commands for working in the ChemSketch window in Structure mode.

General toolbar located right below the menu bar includes tools that are present in both Structure and Draw modes and will help you with tasks relevant to both modes such as: saving, opening

files, undoing/redoing operations, copying and pasting, zooming in and out, as well as inserting various templates.

Structure toolbar placed below the General toolbar and only present in the Structure mode. This contains tools for drawing and manipulating chemical structures, as well as buttons that link you to additional modules (see section 1.2).

Atoms toolbar displayed vertically to the left of the screen contains buttons representing atoms, as well as tools for changing atom properties (charge, valence, numbering, etc.).

Reference toolbar placed to the right of the window contains the Table of Radicals and various buttons representing ready-made radicals you take from the table. You can also access ACD/Dictionary from this toolbar.

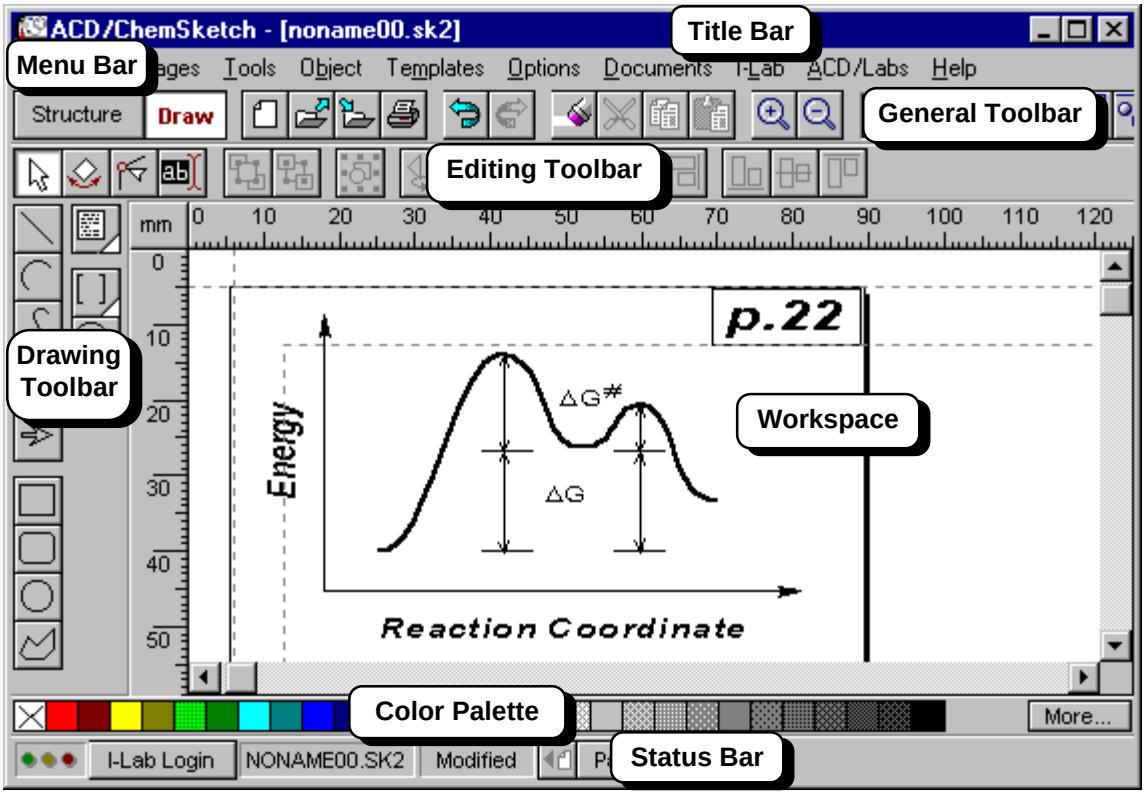
Workspace is the open area in the middle where structures are drawn. (Sample shown.)

Color Palette at the bottom of the workspace allows you to quickly color atoms and bonds in the selected chemical structures (by clicking or right-clicking on the colors).

Status bar contains information that may be useful for the current moment: name of the SK2 file you are working on, page number in the SK2 file, number of fragments in the workspace, molecular formula of the selected structure, as well as one of the available chemical properties for the selected structure. It also contains a button for automatic I-Lab access.

2.3.2 Draw Mode Screen

Below you can see the screen with the Draw Mode enabled. Please, pay attention to the names and position of the toolbars, since we are going to use these terms throughout the whole guide.



Title bar shows the name of the program and the name of the currently open file. The default file name is NONAMExx.SK2, where 'xx' is a counter.

Menu bar contains a series of words. Each word links to a list ('menu') of related commands for working in the ChemSketch window in Draw mode.

General toolbar located right below the menu bar includes tools that are present in both Structure and Draw modes and will help you with tasks general for both modes such as, saving, opening files, undoing/redoing operations, copying and pasting, zooming in and out, as well as inserting various templates.

Editing toolbar placed below the General toolbar and only present in the Draw mode incorporates tools for editing and manipulating drawn graphical objects.

Drawing toolbar displayed vertically to the left of the screen contains buttons for drawing various graphical objects and text.

Workspace is the open area in the middle where graphical objects are drawn and text is typed. (Sample shown.)

Color Palette at the bottom of the workspace allows you to quickly color selected objects (by clicking or right-clicking on the colors).

Status bar contains information that may be useful for the current moment: name of the file you are working on, status of the document and page number.

3. Drawing Simple Structures

3.1 Objectives

This chapter considers the basics of structure drawing, which occurs only in Structure Mode. Here you will learn how to:

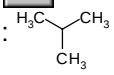
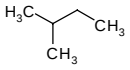
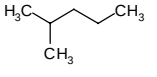
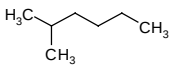
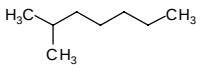
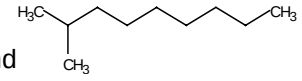
- draw atoms, bonds and labels;
- flip a drawn molecular structure;
- select, rotate and resize drawn structures; and
- clear the screen.

3.2 Drawing Atoms, Bonds and Labels

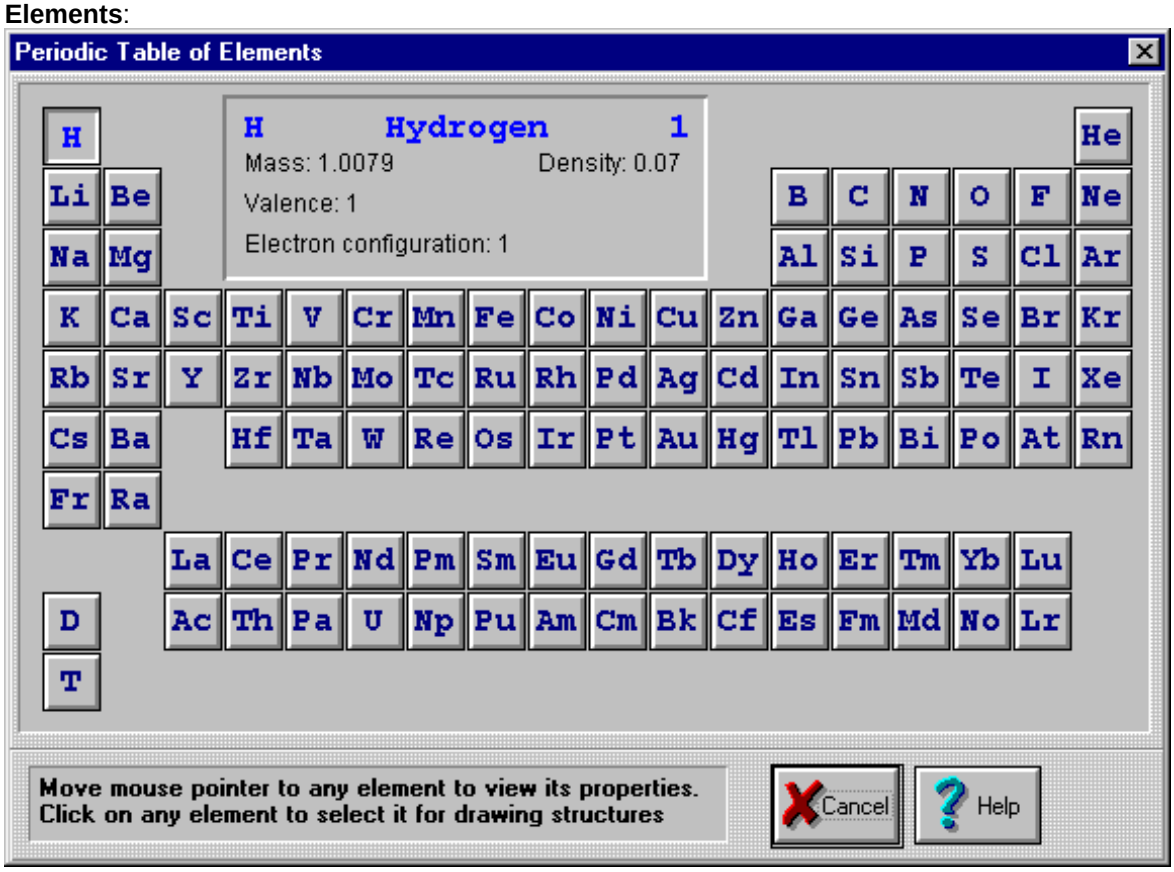
Drawing bonds and atoms is the basic activity in the ChemSketch. Make sure that you are in Structure Mode for all following actions.

3.2.1 Using the Draw Normal Tool

The Draw Normal tool is the default tool when the program is started. In this mode you can easily draw normal or branched chains and replace the drawn atoms with other atoms from the Periodic Table of Elements.

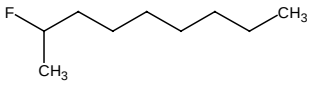
1. Make sure that the **Draw Normal** tool is enabled on the Structure toolbar and that the **Carbon** atom is selected on the Atoms toolbar.
2. Click in an empty space to draw CH_4
3. Click on CH_4 to add a $-CH_3$ group, creating CH_3-CH_3 with a standard bond length. Click twice more on the same Carbon to draw
4. Click the **Set Bond Vertically** button on the Structure toolbar and click on any bond of the structure to rotate it to this orientation: 
5. Click the **Draw Normal** button on the Structure toolbar.
6. Click on the right-most Carbon atom to draw 
7. Repeat the above step to draw the following structures:  ,  ,  and 

8. Click the **Periodic Table** button on the Atoms toolbar to open the **Periodic Table of Elements**:



9. Click the **Fluorine** button in the Periodic Table of Elements. Note that the **Fluorine** button F is added to the Atoms toolbar.

10. Click on the left-most Carbon to replace it with a Fluorine atom:



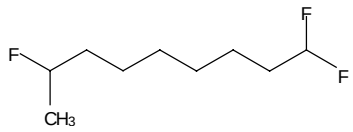
> **Note** When you select new elements from the **Periodic Table of Elements**, corresponding buttons are automatically added to the Atoms toolbar. To remove these buttons from the Atoms toolbar, double click on any of them or double click on the Atoms toolbar and choose **Yes**.

3.2.2 Using the Draw Continuous Tool

When the Draw Continuous tool is active, bonds can only be drawn from the highlighted atom. To highlight an atom, click on it. This mode is very convenient for "sprouting" new atoms from a selected atom.

1. Click the **Draw Continuous** button on the Structure toolbar. Alternatively, you can press the right mouse button to switch to this drawing mode.
2. Make sure that the **Fluorine** button F is selected on the Atoms toolbar.

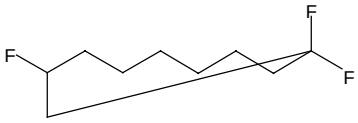
3. Click on the right-most carbon in the drawn structure to select it. Click the second time to sprout fluorine from the selected carbon. Click twice on the same carbon again to sprout the second fluorine atom:



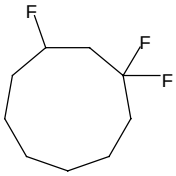
3.2.3 Using Mouse Drag

With either drawing tool, **Draw Normal** or **Draw Continuous** , dragging the mouse from one atom to another draws a single bond between them. If you drag to or from an empty space, a new atom is inserted at the start or at the end of the drawn bond.

With either the **Draw Normal** or **Draw Continuous** tool active, point the mouse arrow to one of the terminal carbons and drag to another terminal carbon to draw the following structure:



3.2.4 "Cleaning" the Structure

1. Click the **Clean** button on the Structure toolbar to standardize all the bond lengths and angles in the drawn structure to obtain the following: 

> **Note** The **Clean** command not only standardizes all bond lengths and angles to make the structure look nice — it makes the drawn structures closer to being chemically correct. For acyclic fragments, for example, it places the bonds near the sp^2 carbons at 120^o angles and the bonds near the sp carbon at 180^o (linear). If you draw geometrical and stereo isomers, the "Clean" command standardizes their bond lengths and angles while retaining all of their structural significance.

3.2.5 Using the Stereo, Coordinating and Undefined Bond Tools

You can draw a wide variety of bonds, besides the "ordinary" connection:

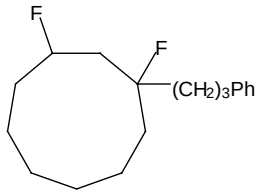
- stereo bonds directed away from you ;
- stereo bonds directed towards you ;
- coordinating bonds ;
- and undefined bonds .

Select any of these tools and click on any bond in the drawn structure. Click repeatedly on a stereo or coordinating bond to change its direction.

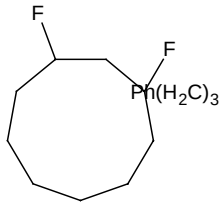
3.2.6 Editing Atom Labels

The **Edit Atom Label** tool allows you to substitute terminal atoms with shorthand abbreviations.

1. Click the button on the Atoms toolbar and then on the right-most fluorine atom in the drawn structure.
2. In the Edit Label dialog type **(CH2)3Ph** and click the **Insert** button. Note that the label is inserted in the desired position and the indexes are automatically subscripted:

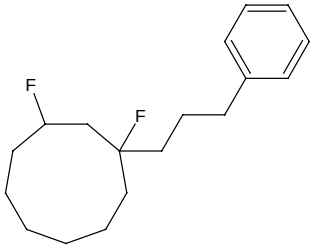


3. Select the **Change Position** tool and click on the label to invert it:



> **Tip** If you click on the label with the **Change Position** tool active while holding down the SHIFT key, the connection point of the label will be changed.

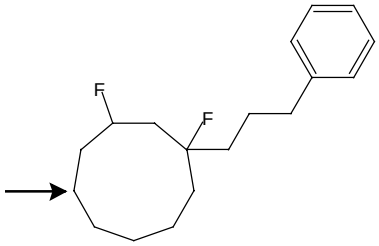
4. With the active **Edit Atom Label** tool click on the obtained shorthand abbreviation to open the **Edit Label** dialog box again. Then click on the **Expand** button to obtain the following structure:



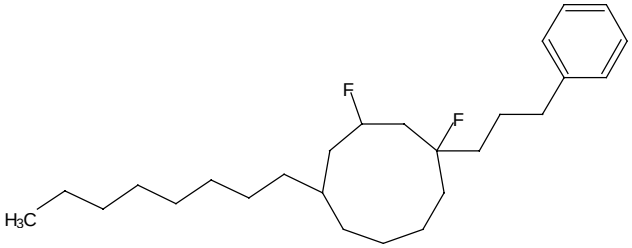
3.2.7 Using the Draw Chains Tool

Using the **Draw Chains** tool, you can easily draw short or long chains with a single click and mouse drag.

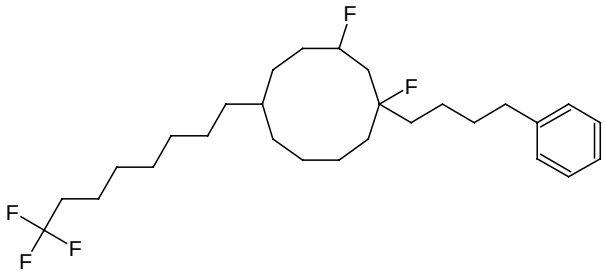
1. Click the **Draw Chains** button on the Structure toolbar and point the mouse arrow to the atom indicated by the arrow:



2. Press mouse button and drag to the left side. As you move the mouse away from the structure, a carbon chain is created. Note the carbon counter (C #) located beside the mouse arrow changes with each carbon added or removed. Continue until the counter reaches C 8, then release the mouse button to finish the chain:



3. With the active **Draw Chains** tool select the **Fluorine** button on the Atoms toolbar and click on the left-most carbon to sprout three fluorine atoms. Then click on the **Clean** button on the Structure toolbar to obtain the following structure:



3.3 Flipping Structures

You can rotate or flip the structure(s) by using the following buttons:

Button	Function
	Select this button and then click on the bond to set it horizontally, rotating the rest of the structure correspondingly.
	Select this button and then click on the bond to set it vertically, rotating the rest of the structure correspondingly.
	Flips the structure around the clicked bond.
	Flips selected structure or fragment (or if nothing is selected, all drawn structures) from top to bottom.
	Flips selected structure or fragment (or if nothing is selected, all drawn structures) from left to right.

3.4 Selecting, Rotating, and 3D Rotating

You can select atoms, bonds and fragments in two different ways, by using the button which toggles between

- the **Lasso Selector** or
- the **Rectangle Selector** .

Once the fragment(s) has been selected, there are three ways you can move it:

- **Move** ,
- **Rotate/Re-size** ,
- **3D Rotate** ,

or you can perform one or more other operations on it:

- **Delete** ,
- **3D Optimization** . or
- **2D Optimization** (or **Clean**) .

3.5 Clearing the Screen

To clear the screen, you can do one of the following:

Choose the **New** command from the **File** menu to open a new document.

Choose the **New Page** button from the upper left set of buttons to go to a new page.

Choose the **Select All** command from the **Edit** menu and then choose the **Delete** command.

Click the **Delete** button on the General toolbar. Click on an empty space away from the drawn structure to select all of the structures, then click on any structure to delete the entire screen.

4. Drawing More Complex Structures

4.1 Objectives

Now that you have studied the basics of structure drawing described in the previous chapter you may continue with drawing more complex structures using advanced tools of ChemSketch.

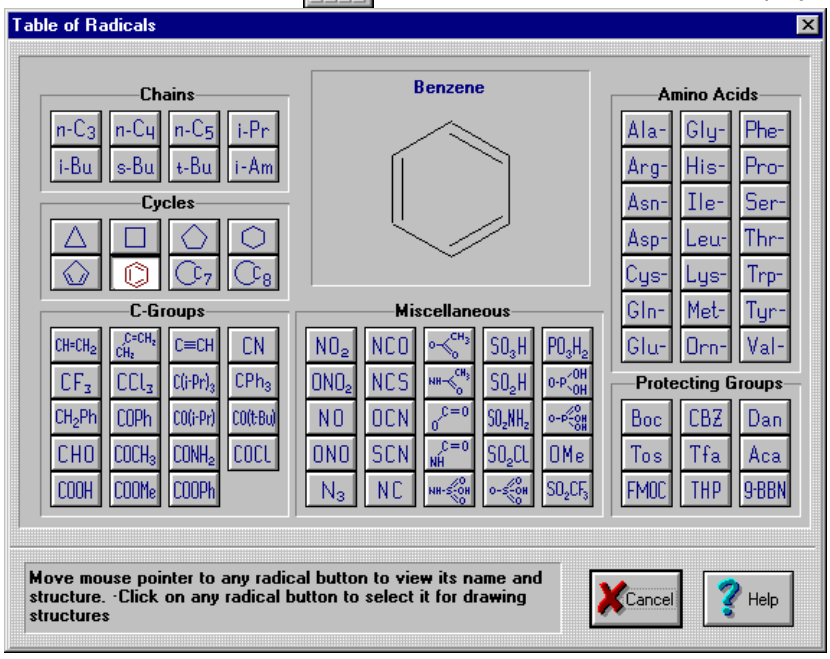
In this chapter you will learn how to:

- use the Table of Radicals for drawing typical radicals;
- quickly draw ring structures;
- delete and replace atoms;
- set double and triple bonds;
- set an atom's charge, draw cations and anions; and
- change various atomic properties.

4.2 Using the Table of Radicals

The **Table of Radicals** includes pre-drawn structures of amino acids, their protecting groups, as well as nucleotides and other frequently used radicals.

1. Clear the screen using the directions given in previous section.
2. Click on the **Table of Radicals** button on the **References** toolbar to display the radicals:

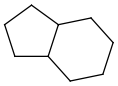
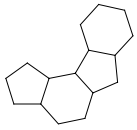
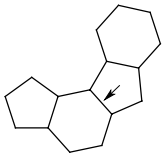
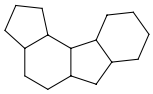
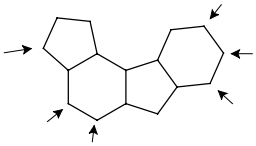


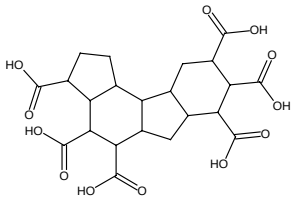
3. Click the **Cyclohexane** button in the Table of Radicals.

4. A **Cyclohexane** button is now located and currently selected on the References toolbar on the right side of the screen.
5. Repeat these steps for the **Cyclopentane** button .

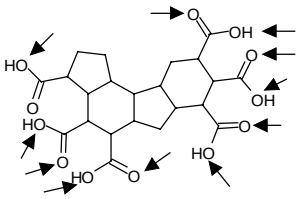
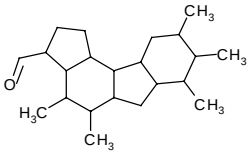
> **Note** When you select new radicals from the Table of Radicals, the corresponding buttons are automatically added to the References toolbar. **To remove these buttons** from the References toolbar, double click on any of them or double click on the **References** toolbar and choose **Yes**.

4.3 Using Ring Structures

1. Select the cyclopentane button on the **References** toolbar on the right side. Click on the screen to create a five-membered ring.
2. On the same toolbar, select the icon. Now point the mouse arrow to highlight the indicated bond, and click to create the following structure: 
3. Repeat these steps to create the following structure; 
4. Click the **Set Bond Vertically** button then click on the indicated bond  to rotate the structure around this bond to obtain the following: 
5. Click the **Table of Radicals** button on the References toolbar.
6. In the **Table of Radicals** window, select the carboxyl group by clicking the button.
7. Click on the atoms indicated in  to sprout carboxyl groups from them:



4.4 Deleting Atoms and Fragments

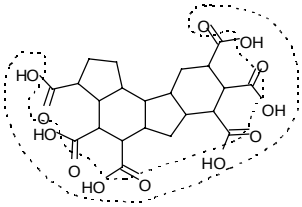
Delete the atoms indicated by arrows in  to draw 

You can do this in two ways: delete each atom individually or delete all atoms simultaneously.

4.4.1 Deleting Atoms Individually

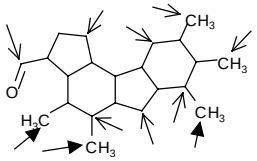
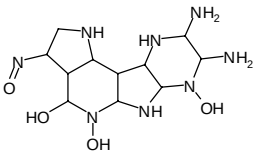
1. Click the **Delete** button .
2. Click each of the atoms which you want to delete.

4.4.2 Deleting All Atoms Simultaneously

1. Click the **Lasso On/Off** button on the Structure toolbar to enable the **Lasso** selection mode . Note the **Select/Move** tool becomes active.
2. Drag to include all of the specified atoms in the closed Lasso line:
3. Click on the **Delete** button on the General toolbar. 
4. Click on any of the highlighted atoms to delete all of them simultaneously.

> **Note** You can select atoms, bonds and fragments in two different ways, by using either the **Lasso** selector or the **Rectangle** selector . To deselect fragment(s), click anywhere on an empty space.

4.5 Replacing Atoms

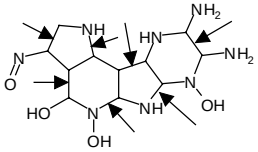
Replace the atoms indicated with arrows in  to draw 

1. Click the **Nitrogen** button on the left Atoms toolbar and then click on all the carbons denoted by an open-head arrow on the above structure.
2. Click on the **Oxygen** button on the Atoms toolbar and then click on three Carbons denoted by a solid-head arrow.

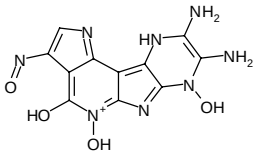
> **Note** You cannot replace atoms with the **Draw Continuous** tool (see Section 3.3).

4.6 Setting Double and Triple Bonds

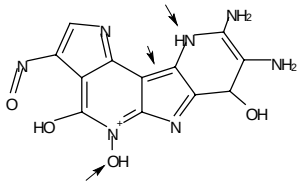
1. With any one of the **Draw Normal**, **Draw Continuous** or **Draw Chains** tool active, click on the bonds indicated in



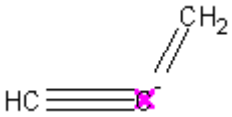
to set double bonds:



2. Using the **Change Double Bond or Hydrogen Position** button the structure's appearance can be "fine-tuned". Select this button and click on the indicated hydrogens and double bonds. Note the movement of hydrogen around the nitrogen and oxygen, and the double bond around the single bond:



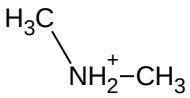
Note You can set a double or triple bond or reset a single bond by repetitive clicking on a chosen bond. This will cycle through all bond orders available. When an atom has an invalid number of bonds, a corresponding charge is placed on it and it is crossed out with a red "X":



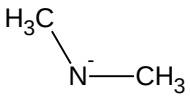
If you want to disable the crossing-out function, select the structure, choose **Structure Properties** from the **Tools** menu, clear the **Cross Out Invalid Atom** check box in the **Common** tab and click **Apply**.

4.7 Setting Charges and Defining Anions and Cations

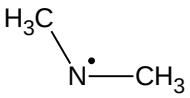
In this section we will draw the following set of structures:



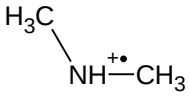
anion



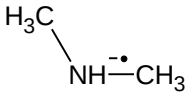
cation



free radical

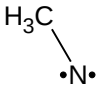


radical cation



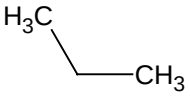
radical anion

singlet biradical

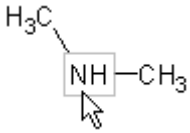


triplet biradical

1. Choose the **Carbon** button [C] on the Atoms toolbar and make sure that the **Draw Normal** tool [/] is on. Click three times in one place to draw the following structure:



2. Choose the **Nitrogen** button [N] and click on the middle carbon in the fragment to replace it with a nitrogen:



3. Click the bottom right triangle of the [+] button on the left Atoms toolbar to expand it to the following group:

   [+] Increment Charge;

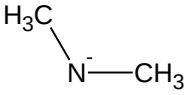
   [−] Decrement Charge;

   [•] Radical;

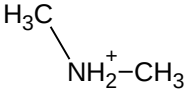
   [+•] Radical Cation;

   [−•] Radical Anion.

4. Click on the **Decrement Charge** button [−] and then click on the NH group to make an anion:

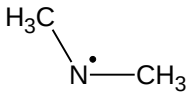


5. Right-click to switch to the **Increment Charge** tool (or choose [+] from the group of buttons) and click twice to make a cation:

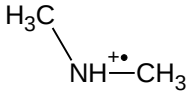


> **Note** When you use the **Charge** buttons, [+] or [−], to change the charge of a non-metal, the corresponding number of hydrogen atoms is automatically added to it, or removed from it, to preserve proper chemical valency. If you change the charge of a metal, the charge is changed in increments or decrements in accordance with the next chemically valid charge of the corresponding ion. (You can view common valences used in the **Periodic Table of the Elements**.)

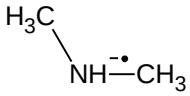
6. Choose the **Radical** button [•] from the group of buttons shown in step 4 above and click on the NH_2 group to draw a free radical:



7. Right-click in an open part of the workspace to quickly switch to the **Radical Cation** tool or choose the corresponding button [+•] and click to draw the radical cation:

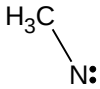


8. Right-click in an open part of the workspace to switch to the Radical Anion tool [−•] and click to draw the radical anion:

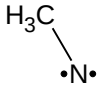


9. Choose the **Delete** button [ ] on the top General toolbar and click the right CH_3 group to delete it.

10. From the group of buttons in step 4 choose the **Radical** tool [•] and click on the NH group several times until the following singlet biradical is obtained:



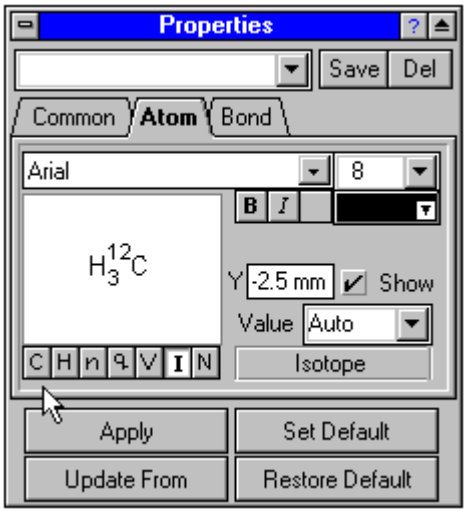
11. Continue clicking with the radical tool until the triplet biradical is displayed:



4.8 Changing Atom Properties

If you want to display the valency or the isotopic mass of the atom in a ChemSketch structure—or even change the typeface or the size of the atom, you should use the Properties panel.

1. Click the **Select/Move** button .
2. Double-click on the atom whose displayed properties you want to change. This will make the **Properties** dialog box appear. Switch to the **Atom Properties** tab:



3. Clicking the buttons

displays options for changing
   - **C** – atom symbol,
   - **H** – attendant hydrogens,
   - **n** – index of the attendant hydrogens,
   - **q** – charge,
   - **V** – valence,
   - **I** – isotopic mass,
   - **N** – numbering of atom in the overall molecule.
4. As you set the values, click **Apply** to have the change appear immediately on the selected atom.

5. Advanced Structures and Reaction Schemes

5.1 Objectives

This chapter is the next step to drawing much more complicated structures as compared to the one described in the previous chapters. If you are using ChemSketch for the first time, it is recommended that you do the exercises described here only after completing the previous chapters.

Here you will learn how to:

- draw structures of cyclic Alkanes and Peptides using the 2D optimization (Clean Structure) tool;
- use the 3D Optimization tool for drawing “spectacular” 3D structures of Bicyclo[2.2.2]octane, tripticene, cubane and dodecahedrane;
- draw reaction schemes.

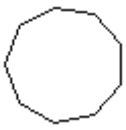
5.2 2D Optimization

The Clean option can be considered to be a 2D-optimization of the drawn structure, *i.e.* re-drawing and re-sizing it to standardize all the bond lengths and angles. Using this option you can easily draw a structure perfectly. Some examples:

5.2.1 Creating the Structure of Cyclic Alkanes

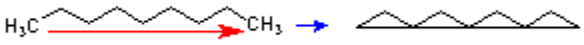
This section is based on the movie **cycloalk.exe** which can be downloaded from our web site or found in the Movies folder.

Using the following technique you can quickly draw cyclic alkanes perfectly. Here's how to draw **Cyclononane**:

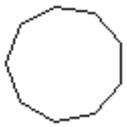


1. Switch to the Structure mode and delete any previously drawn structures by pressing CTRL+A and then DELETE.
2. Choose the **Draw Chains** tool and drag in the workspace to draw a 9-member chain. Note that the informative cursor shows the number of atoms in the chain.

3. Click on the right mouse button to quickly switch to the **Draw Normal** tool and drag from one end atom to another in order to connect them with a bond.



4. Click on the **Clean Structure** button to obtain the following structure:

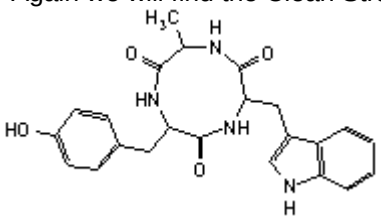


Try to draw C_{10}- and C_8-rings using the above technique.

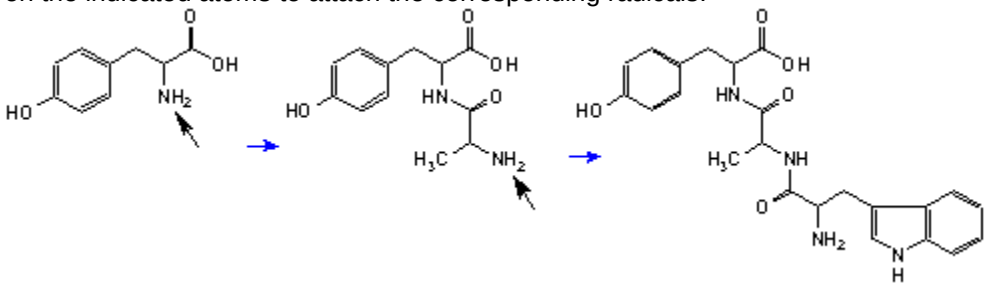
5.2.2 Creating the Structure of a Cyclic Peptide

This section is based on the movie **pept.exe** which can be downloaded from our web site or found in the Movies folder.

Let's draw the cyclic Tyr-Ala-Trp. Again we will find the Clean Structure button is useful.

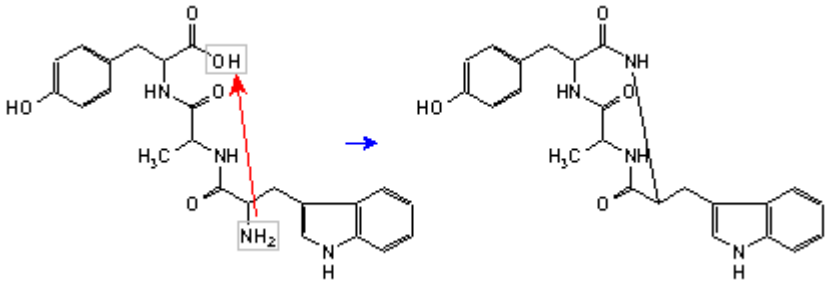


1. Switch to the Structure mode and delete any previously drawn structures by pressing CTRL+A and then DELETE.
2. From the **Template Window** choose the Amino Acids tab.
3. From the set of amino acids, choose **Tyrosine** and click in the workspace to copy the structure.
4. From the **Table of Radicals** choose **Alanine** Ala- and then **Tryptophan** Trp- and click on the indicated atoms to attach the corresponding radicals:

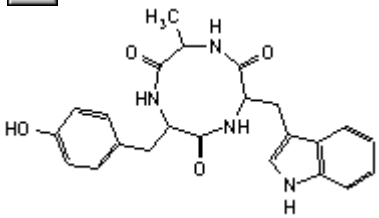


> **Note** You can flip the template shadow before fixing it by pressing the TAB key.

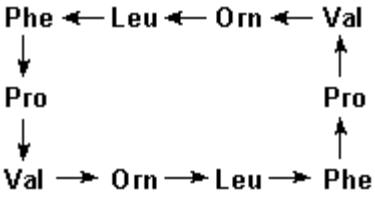
5. Click the right mouse button to quickly switch to the **Select/Move** tool and drag the NH2 group to the OH group as shown:



6. Click on the **Clean Structure** button to obtain the following structure:



Try to draw any other cyclic peptide, for instance Gramicidine S:



5.3 3D Optimization

This section explains how to create structures that have “realistic” angles and bond lengths. There is no need to explain how difficult it is to draw such molecules proportionally. The 3D-Optimization and 3D Rotation options will help you to quickly cope with this task. These options make it possible to create complex structures in ACD/ChemSketch with ease.

The 3D optimization algorithm is a proprietary version of molecular mechanics with the force field initially based on CHARMM parameterization[1]. The modifications involve some simplification and were intended to increase the stability and speed of computation. Note that 3D-optimizer is NOT a full-scale molecular mechanics engine. Its design aims to reliably reproduce reasonable conformations from (possibly very unreasonable) 2D drawings, rather than to precisely optimize 3D structures.

If 3D-optimizer produces the conformation different from what you have expected, do not be surprised. It is the very essence of conformational analysis that molecules typically have many conformations. The optimizer finds only one, and it may not be one you expect. For example, you probably expect a cyclohexane fragment to be a chair, but the optimizer may generate twist-boat, which is also one of its suitable conformations (indeed, in many structures this fragment exists in

[1] B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, and M. Karplus. CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. J. Comput. Chem. 4 187-217 (1983).

a twisted form). In such a case, you may try to correct the conformation (e.g., by manually moving the atoms into desired direction and 3D-optimizing the structure again).

You may wish to perform actual conformational analysis of your molecule using a special molecular mechanics or quantum chemistry geometry optimization package. The ChemSketch 3D-optimized structure will serve as input data.

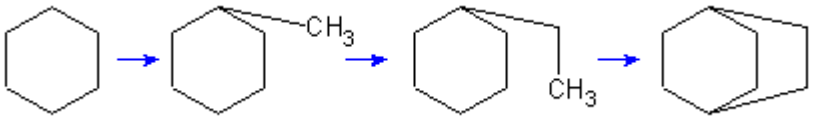
> **Important** Prior to starting any of the exercises in this section, clear the **Add Hydrogens** check box in the **Structure** Tab in the **Preferences** dialog box (**Options** menu).

5.3.1 Creating Structure of Bicyclo[2.2.2]octane

This section is based on the movie **bicyc.exe** which can be downloaded from our web site or found in the Movies folder.

Switch to the Structure mode and delete any previously drawn structures.

1. From the **Table of Radicals** choose **Cyclohexane**. Click in the workspace to place a cyclohexane ring.
2. Click the **Draw Normal** tool and draw the hydrocarbon bridge by dragging as shown in the following scheme:



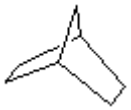
3. Click the **3D Optimization** button to obtain a 3D model of the drawn structure.

> **Note** If there is more than one structure in the workspace you should select the structure you want to 3D-optimize using any of the selection tools (**Select/Move**, **Select/Move/Re-size** or **3D Rotation** tools).

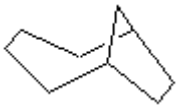
4. If the **Switch to 3D Rotation mode** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu) is selected, you will be automatically switched to 3D Rotation mode after the 3D Optimization is completed. If you are not, switch to the **3D-Rotation** tool. Place the mouse cursor over any atom or bond in the structure and drag the mouse over the workspace to rotate the structure until it is placed as shown:

Note You can choose whether the background bond should be broken or not by selecting or clearing the **Enable bonds intersections** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu).
You can change the position of intersecting bonds by applying the **Bring Bond to Front** or **Send Bond to Back** commands (**Options** menu) to the selected bond.
You can also bring the background bond to the front by clicking on it with the **Change Position** tool active while holding down the SHIFT key.

Try to draw the following structures on your own using the above technique



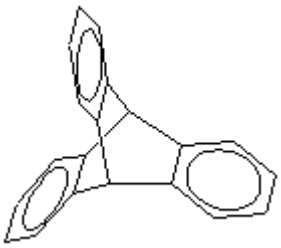
Bicyclo[2.2.1]heptane



Bicyclo[4.2.1]nonane

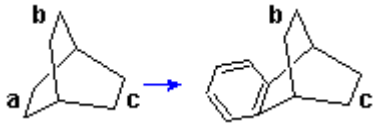
5.3.2 Creating the Structure of Triptycene

This section is based on the movie **triptyc.exe** which can be downloaded from our web site or found in the Movies folder.

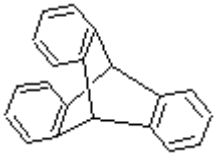


Switch to the Structure mode and delete any previously drawn structures by pressing **Ctrl + A** and **Del**.

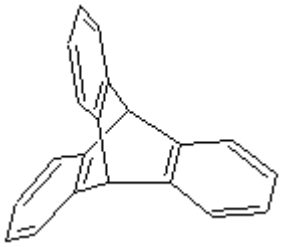
1. Draw the structure of **bicyclo[2.2.2]octane** as described above or use the corresponding template from the **Template Window** (the Bicyclics tab).
2. From the **Table of Radicals** choose **Benzene** .
3. Position the cursor over the bond **a** and click to attach the benzene ring to this bond:



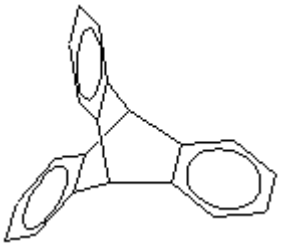
4. Repeat steps 2--3 for bonds **b** and **c** to obtain the following structure:



5. If there is more than one structure in the workspace, select the structure you want to 3D-optimize using any of the selection tools (**Select/Move** , **Select/Rotate/Re-size** or **3D Rotation** tools)
6. Click on the **3D Optimization** button to obtain a 3D-model of the drawn structure:

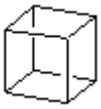


7. If the Switch to **3D Rotation mode** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu) is selected, the program will automatically switch to 3D Rotation mode after the 3D Optimization is completed, if it does not, select the **3D Rotation** tool . Place the mouse cursor over any atom or bond of the structure and drag the mouse over the workspace to obtain the projection you want.
8. Choose the **Show Aromaticity** command from the **Tools** menu to show the aromatic rings:



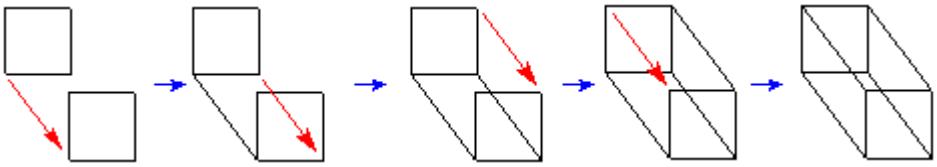
5.3.3 Creating the Structure of Cubane

This section is based on the movie **Pr_cub.exe** which can be downloaded from our web site or found in the Movies folder.

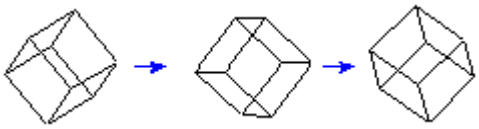


1. Switch to the

mode and delete any previously drawn.
2. From the **Table of Radicals** choose **Cyclobutane** . Click twice in the workspace to place two 4-membered rings one under another.
3. Choose the **Draw Normal** tool and connect the corners of cyclobutane molecules with bonds by dragging from one atom to another as shown:



4. Click on the **3D Optimization** button to obtain the 3D model of the drawn structure.
5. Select the 3D Rotation tool if it is not already selected.
6. Place the mouse cursor over any atom or bond of the structure and drag the mouse over the workspace to obtain the projection you want:



Note You can choose whether the background bond should be broken or not by selecting or clearing respectively the **Enable bonds intersections** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu).

You can change the position of intersecting bonds by applying the **Bring Bond to Front** or **Send Bond to Back** commands (**Options** menu) to the selected bond. You can also bring the background bond to front by clicking on it with the **Change Position** tool active while holding down the SHIFT key.

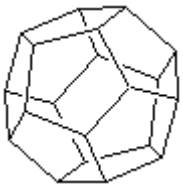
Try to draw the following structures on your own using the above technique

Prismane

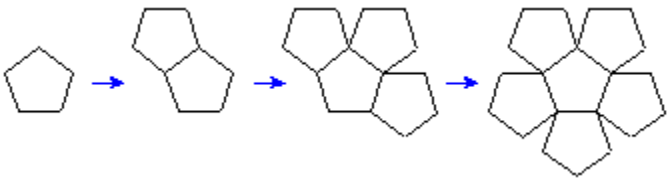
Hexacyclo[4.2.0.0^{2,5}.0^{3,9}.0^{4,8}.0^{7,10}]decane

5.3.4 Creating the Structure of Dodecahedrane ([5]Fullerene-C_{20})

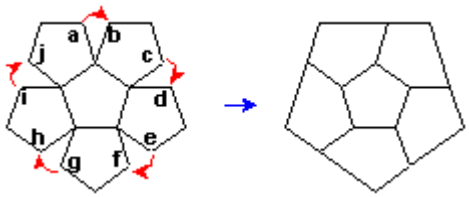
This section is based on the movie **fuller.exe** which can be downloaded from our web site or found in the Movies folder.



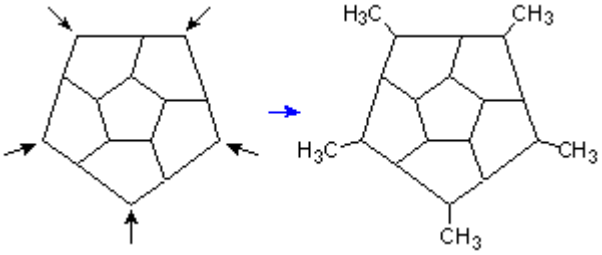
1. Switch to the Structure mode and delete any previously drawn structures.
2. From the **Table of Radicals** choose **Cyclopentane**. Click in the workspace to place a cyclopentane ring.
3. Consequently position the mouse pointer over every bond of the ring and click to attach five other rings:



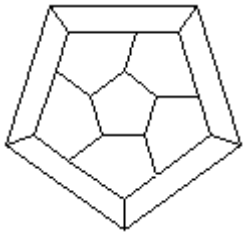
4. Click the right mouse button to quickly switch to the **Select/Move** tool .
5. Move by dragging atoms **a**, **c**, **e**, **g**, **i** to atoms **b**, **d**, **f**, **h**, **j** accordingly as shown in the following scheme to merge them:



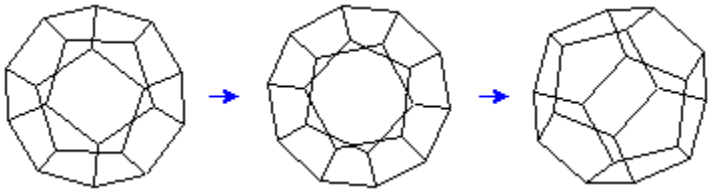
6. Select the **Carbon** button C on the left Atoms toolbar and click directly on the points indicated by arrows to add more atoms and bonds:



7. Connect the adjacent methyl groups with single bonds by dragging from one terminal atom to another to obtain the following structure:

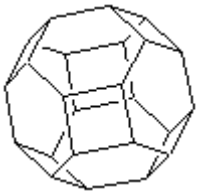


8. Click on the **3D Optimization** button to obtain the 3D model of the drawn structure.
9. Select the **3D Rotation** tool . Place the mouse cursor over any atom or bond in the structure and drag the mouse over the workspace to obtain the projection you want.

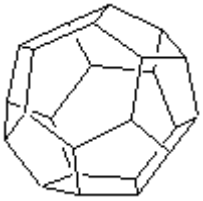


> **Note** You can choose whether the background bond should be broken or not by selecting or clearing respectively the **Enable bonds intersections** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu).
>
> You can change the position of intersecting bonds by applying the **Bring Bond to Front** or **Send Bond to Back** commands (**Options** menu) to the selected bond. You can also bring the background bond to front by clicking on it with the **Change Position** tool active while holding down the SHIFT key.

Try to draw the following structures using the technique described above



[4,6]Fullerene-C_{24}

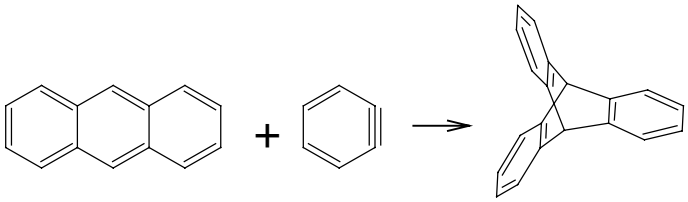


[5,6]Fullerene-C_{24}

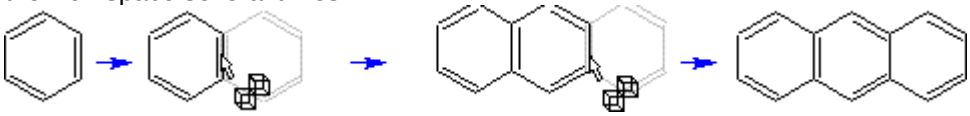
5.4 Drawing a Reaction Scheme

This section is based on the movie **reaction.exe** which can be downloaded from our Web site or found in the Movies folder.

In this section we will draw the following scheme:

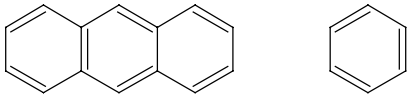


1. From the **Table of Radicals** choose **Benzene** (if you have previously used this template recently, it can found in the right Reference toolbar).
2. Press the TAB key to flip the template shadow and draw the following structure by clicking in the workspace several times:

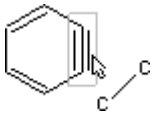


> **Note** To draw a fused-ring structure, place the cursor directly over a ring bond and click.

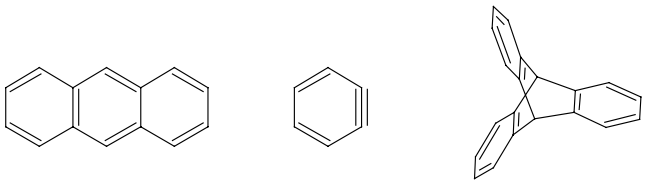
3. Press TAB to flip the shadow again and click beside the drawn structure to place a separate ring. Right-click to hide the template shadow.



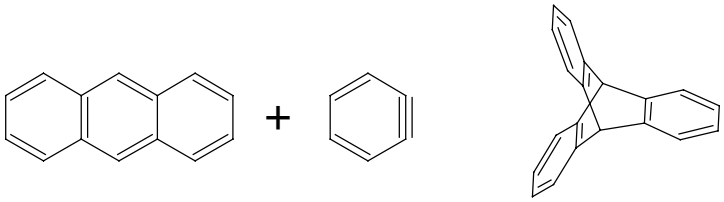
4. Click the **Draw Normal** tool on the upper Structure toolbar and click on the bond of the ring to make it triple:



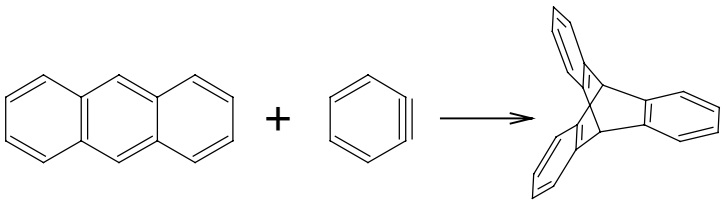
5. Draw the structure of Triptycene as described in section 5.3.2 and place it beside the other drawn structures:



6. From the Structure toolbar choose the **Reaction Plus** tool and click between the first and the second structures to place it:



7. Click the **Reaction Arrow** tool and click or drag to place it as well:



> **Note** By clicking the bottom right triangle of the **Reaction Arrow** button you can choose among various type of arrows. Some arrows are treated as graphical objects, however, and may not export properly.

8. To move the plus sign or the arrow, click the **Select/Move** tool , point to the object and drag.

6. Advanced Drawing: Templates

6.1 Objectives

This chapter will bring you one step closer to an advanced drawing expert once you have mastered the powerful Template feature. You will learn:

- some ways template usage can help you;
- how to apply the Instant Template tool for drawing structures containing repetitive fragments;
- more ways of using the Table of Radicals;
- how to use the Template Window for drawing DNA molecules and complex biomolecules;
- how to create your own templates; and
- what templates are available from our Web site.

6.2 Overview

ACD/ChemSketch includes the following 3 sources of structure templates:

- Table of Radicals ;
- Template Window ;
- Instant Template tool .

While the binding point of any template in the **Table of Radicals** is fixed (invariable), the **Template Window** and the **Instant Template** tool allow you to specify any atom or bond to be the binding point simply by clicking directly on it. However, no matter what the source of template is, the principles of joining are the same. There are several ways of joining the template to a drawn structure:

By fusing the bonds of the structure and template: point the mouse pointer over the bond so that the corresponding bonds of the structure and the template shadow are fused and then click.

By attaching the template to the structure: point the mouse pointer on the corresponding atom on the structure so that the connecting bond appears and click

By drawing a spiro connection between the template and the structure: point the mouse pointer on the atom you want to be the binding point and click holding down the SHIFT key.

> **Note** You can flip the template shadow before fixing it by pressing the TAB key

Template Window Organizer is a very convenient way for managing template files: both those included with the software package, and those which you decide to create. It will just take you a minute to save your document as a template and then quickly find it. Note that the only difference between the template file and a usual file is the fact that you can find the template file in the

Template Window Organizer. Otherwise it is a usual document with the extension *.sk2. By saving files this way there are several advantages:

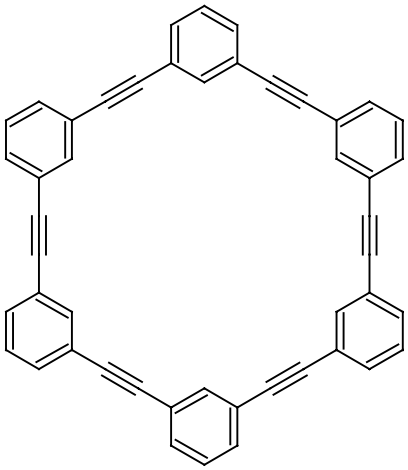
- Your *.sk2 files scattered over different directories and disks will be gathered in one place (the Template Window Organizer).
- You can assign a name to the template that is more descriptive than what the real file name is. This will better reflect the contents of the document and allow you to quickly find the document you need.
- You can quickly find the document by previewing its contents in the Preview Field of the Template Window.
- You can quickly open a selected document from the list just by clicking the Open Document button in the Template Window Organizer.
- Up to 15 templates can be accessed through the Template Window.

6.3 Instant Template Tool

A useful ACD/ChemSketch feature is the Instant Template tool which will help you save time by allowing you to draw fragments quickly. You can think of it as a "replicate" command.

6.3.1 Creating the Structure of a Cyclic Oligomer

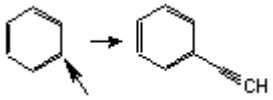
This section is based on the movie **oligomer.exe** which can be downloaded from our web site or found in the Movies folder.



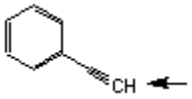
1. Switch to the mode and delete any previously drawn structures by pressing CTRL+A and then DELETE.
2. From the **Table of Radicals** choose **Benzene** . Point the cursor to the upper middle part of the workspace and click to place a benzene ring.

3. From the **Table of Radicals** choose **Ethynyl**

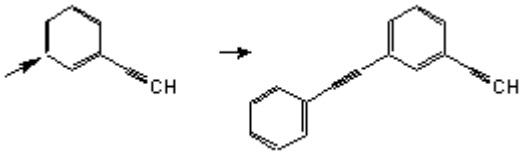
and click on the atom indicated by the arrow to attach it to the ring:



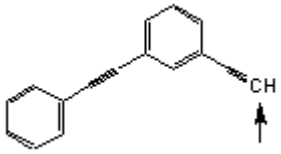
4. Choose the **Instant Template** tool and click on the indicated atom to create an instant template



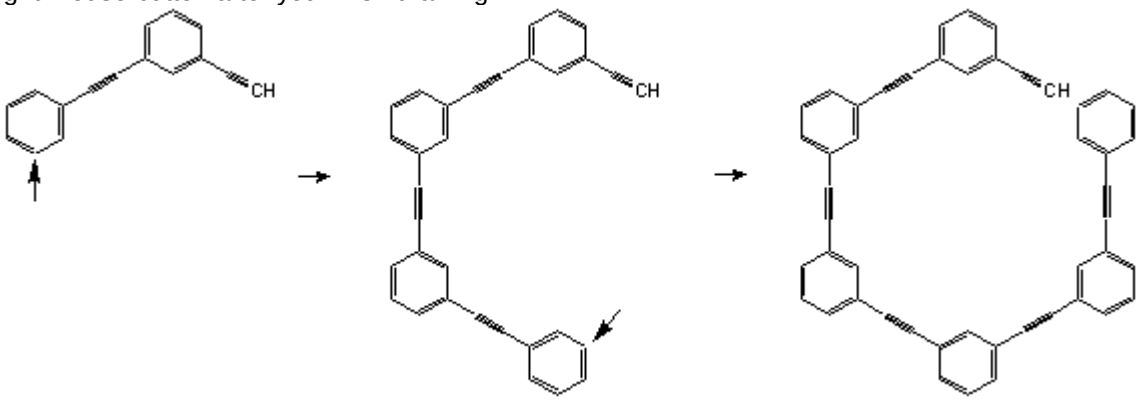
5. Click on the atom indicated by the arrow to attach the template:



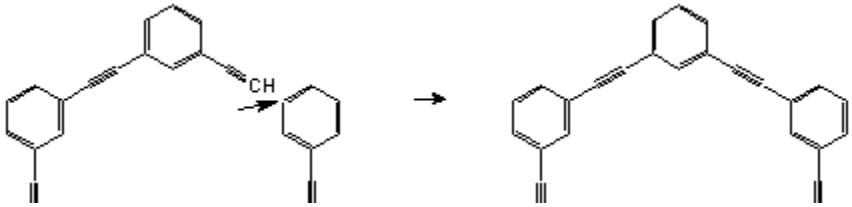
6. Click again and click on the atom to create the template of the whole fragment:



7. Click on the atoms to attach the template as shown. To hide the template shadow click the right mouse button after you finish drawing:



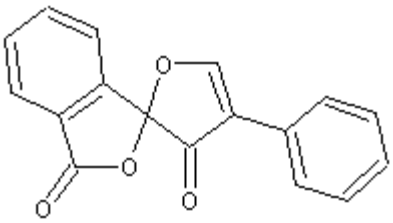
8. Choose the **Draw Normal** tool and click on the indicated atom to complete the ring:



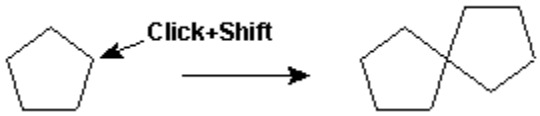
6.4 Table of Radicals in Structure Drawing

6.4.1 Creating the Structure of Fluorescamine

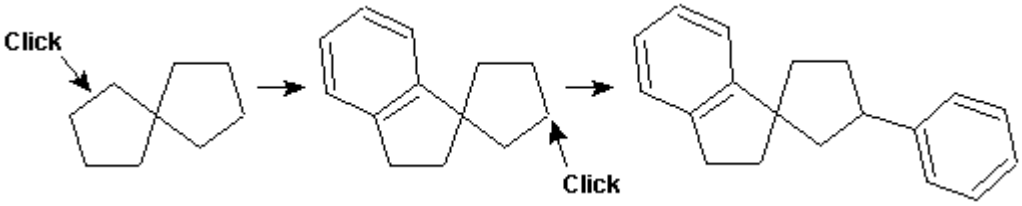
This section is based on the movie **fluor.exe** which can be downloaded from our web site or found in the Movies folder.



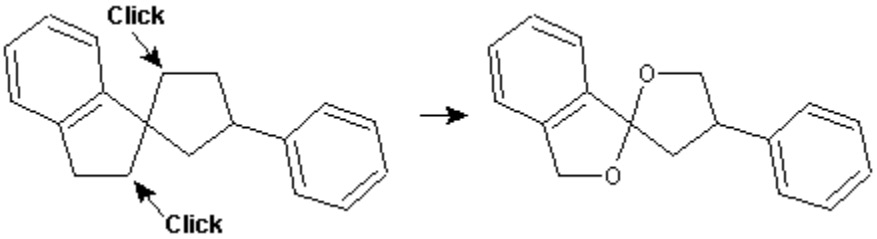
1. Switch to the Structure mode and delete any previously drawn structures.
2. From the **Table of Radicals** choose **Cyclopentane**. Click in the workspace to copy the ring.
3. Click on the indicated atom while holding down the SHIFT key to obtain the spiro-connection with the second cyclopentane ring:



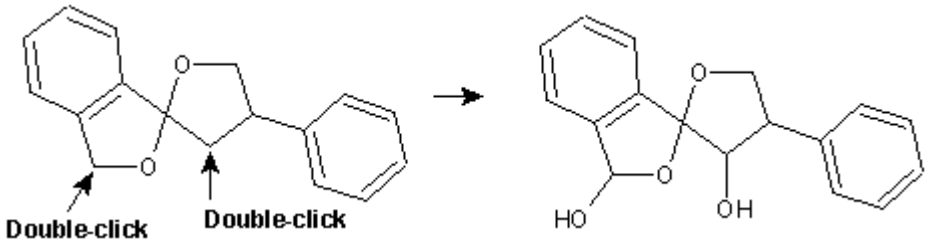
4. From the **Table of Radicals** choose **Benzene**. First click on the indicated bond to fuse the benzene ring and then click on the indicated atom to connect the phenyl radical:



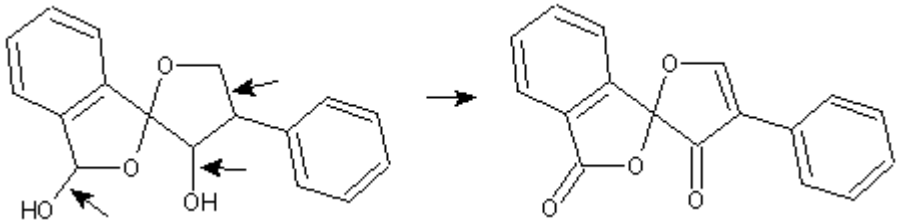
5. Choose the Oxygen button on the Atoms toolbar (note that the **Draw Normal** tool is automatically enabled). Click on the indicated atoms to replace them with oxygen atoms:



6. Click the right mouse button to quickly switch to the **Draw Continuous** tool . Double-click on the indicated atoms to attach the OH groups to them:



7. Click on the indicated single bonds to replace them with double-bonds:

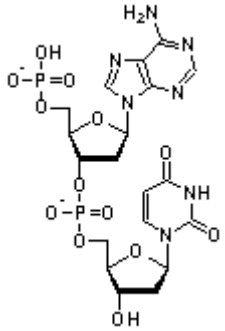


6.5 Templates from the Template Window

A brief tour of available ChemSketch Templates is given in the movie **templ_st.exe** which can be downloaded from our web site or found in the Movies folder.

6.5.1 Creating the Fragment of a DNA Molecule

This section is based on the movie **dna_st.exe** which can be downloaded from our web site or found in the Movies folder.

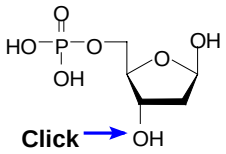


Switch to the Structure mode and delete any previously drawn structures.

6.5.1.1 Drawing the chain of deoxyriboso-5-phosphate fragments

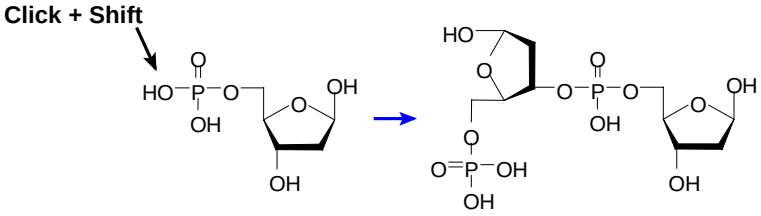
1. Open the **Template Window** . From the

tab choose **2-Dioxyriboso-5-phosphate** (chain form) by clicking on the indicated atom:

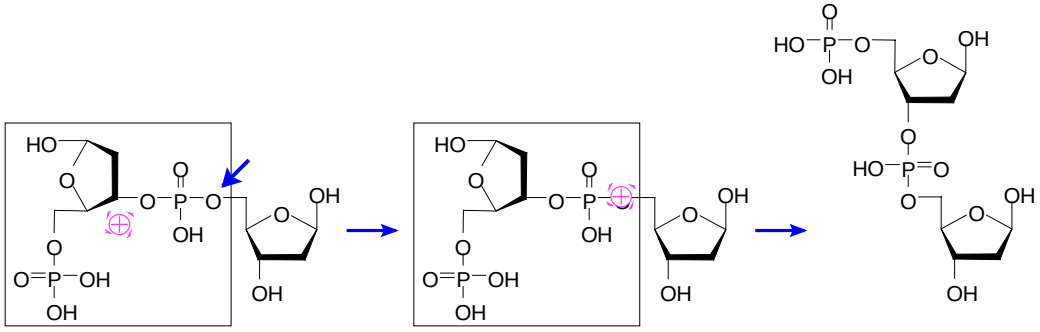


2-Deoxyriboso-5-phosphate

2. Click in the workspace to copy the chosen template.
3. Position the mouse pointer over the indicated atom and while holding down the SHIFT key click to attach the next Dezoxyriboso-5-phosphate fragment:

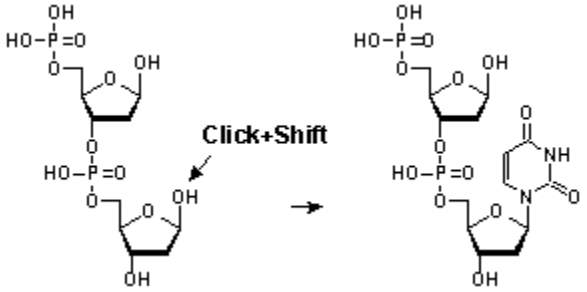


4. Choose the **Select/Rotate/Re-size** tool .
5. Select the indicated part of structure by dragging the selection rectangle around it. Drag the action center onto the oxygen atom indicated by arrow. Then holding down the SHIFT key drag the selected part of structure clockwise to rotate it by 90°:



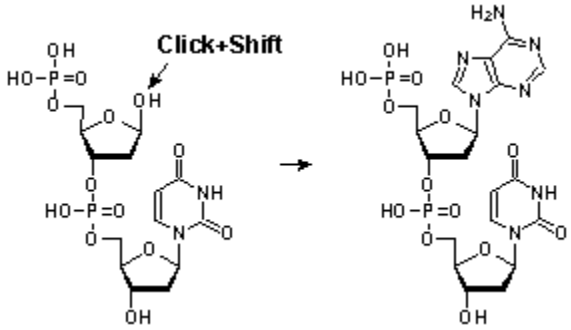
6.5.1.2 Adding the bases

1. Open the **Template Window** . From the DNA/RNA Kit tab choose the base you need by clicking on the atom that will be the attachment point.
2. Position the mouse pointer over the indicated atom and click while holding down the SHIFT key:



> **Tip** You can flip the template shadow before fixing it by pressing the TAB key.

3. Repeat step 2 to add bases to other nucleotides:



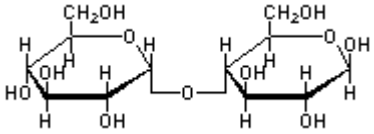
Now try to draw your own DNA or RNA fragment of any other length.

6.6 Drawing Complex Biomolecules

Here are some examples for creating complex biomolecules using different ACD/ChemSketch tools.

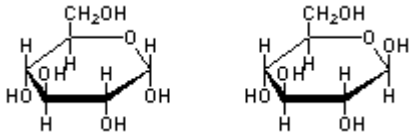
6.6.1 Creating the Structure of β-Maltose

This section is based on the movie **maltose.exe** which can be downloaded from our web site or found in the Movies folder.

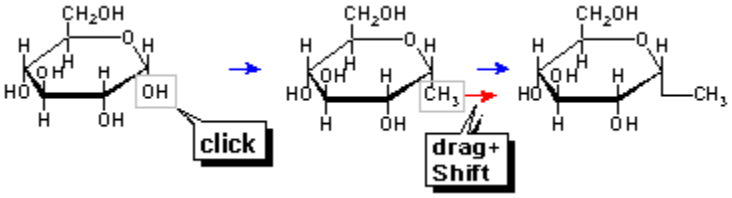


1. Switch to the Structure mode and delete any previously drawn structures.

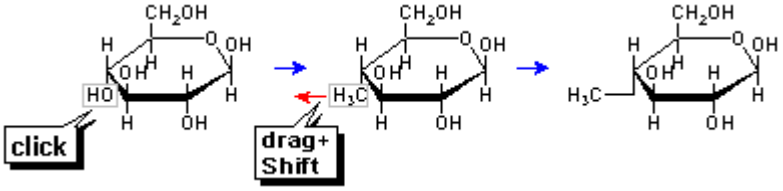
2. In the **Template Window** select the Sugars: alfa-D-Pyr tab, and confirm that you are viewing the Haworth formulae page: 1(4) Haworth Formulae. If not, click on the arrow to the right of the text box and choose accordingly.
3. Click once on **α-D-Glucopyranose** to select it and click in the workspace to copy it.
4. Repeat steps 1-3, but this time select the beta-D-pyranose tab Sugars: beta-D-Pyr and choose **β-D-Glucopyranose**
5. Click in the ChemSketch Window to place it to the right of the first structure.



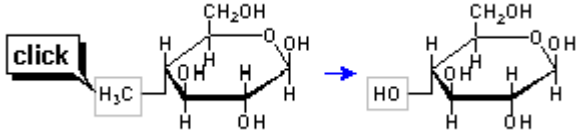
6. Choose the **Carbon** button C. Click on the indicated atom in the **α-D-Glucopyranose** structure to replace it with a CH_3 group and then drag from the CH_3 group to the right while holding down the **Shift** key to draw the bond at a perfect right angle:



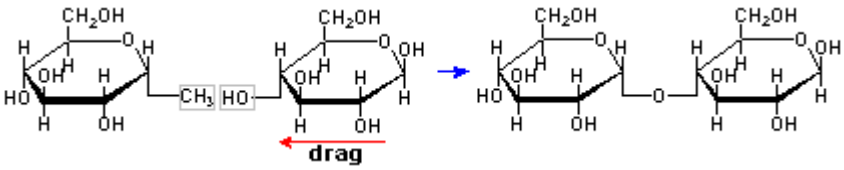
7. Repeat step 3 for the **β-D-Glucopyranose** structure to obtain the following structure:



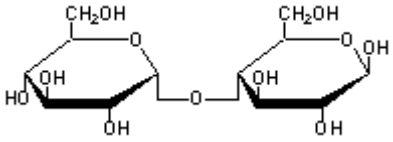
8. Choose the **Oxygen** button O and click on the indicated atom in the **β-D-Glucopyranose** structure:

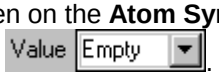


9. Choose the **Select/Move** tool . Click in the workspace adjacent to, but not touching, the **β-D-Glucopyranose** structure to select it. Place the mouse cursor over any atom or bond of the selected structure and drag it to the left until the corresponding OH and CH_3 groups overlap each other:

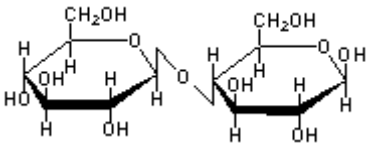


10. If desired, hide single hydrogens in the selected structure by choosing the **Remove Explicit Hydrogens** command from the **Tools** menu:



> **Note** Though the carbon atoms which are bonded to central oxygen are hidden they are still present. If the chemical meaning is important for your task you can remove these atoms in the following way. With the **Select/Move** tool active double click on the hidden atom. When the **Properties** panel appears; click on the tab, then on the **Atom Symbol** button and from the **Value** drop-down list choose **Empty**  . Click **Apply**.

Try to draw the following structure on your own using the technique as described above:



b-Cellobiose

6.7 *Defining a User Template*

It is very easy to assign a ChemSketch file as a Template. As of Summer 1998, we are offering free Templates that can be downloaded from our web site.[2] To designate a ChemSketch file as a template, we recommend you place the SK2 file in the **Templates** folder. Then, do the following:

1. Save your current structures as an SK2 file or open the SK2 file (with structures in it) in ChemSketch.
2. From the **Templates** menu choose the **Save User Template** command.
3. In the **Save User Template** dialog box type in the name for your template, such as “Alkaloids”, and browse to obtain the path name to your file, such as “C:\ACD45\Templates\alkaloids.sk2” and click **OK**.

> **Note** You can enter any name for your document (e.g. for the document b_d_fur.sk2 the following name - Sugars: beta-D-Furanose - would be more appropriate).

Once your document is saved as a user template, its name (under the entered name) is automatically added to the list of templates in the **Template Organizer** and **Template Window** (**Templates** menu).

> **Note** You can create a user template from any document even if it is closed. Open the **Template Organizer** dialog box (**Templates** menu), click the **New...** button, find the needed document and assign it a name.

[2] Check first in the “Templates” folder of the ACD/ChemSketch freeware for the desired template. If you don’t find it there, go to http://www.acdlabs.com/download/download_templates.html .

You can perform the following tasks with the user template:

Quickly find the document and open it for editing. From the Template List (**Template Organizer**) choose the needed template and click **Open Document** button.

Copy any part of your document to the workspace (Structure or Draw mode) without opening the whole document. To do this find your template in the Template List (**Template Window**) and click on the item to place it into the workspace.

6.7.1 The Template.cfg File

The key to management of the templates in ACD/ChemSketch is the file **template.cfg**. This file lets ChemSketch know that a .SK2 file is a template file rather than simply a user file. It can be opened and read with any text editor, although you will likely never need to do so. The Template Window accesses “template.cfg” to let it know what files to display as templates. If a .SK2 file is not shown in the Template Window, it will be added to “template.cfg” by when you open the SK2 as a regular ChemSketch file and select the command to save as a user template.

If **template.cfg** is moved or lost, the **Template Window** will not display any templates. If the template.cfg file is found (by Windows Explorer, for example, or the system “Find File” utility) it can be restored to the default directory or the user’s private directory. If it cannot be found, it must be retrieved by reinstalling ChemSketch or by adding each template individually as detailed above.

6.7.2 Available Templates

As of Summer 1999, this is the list of templates available for download from our “Free Stuff” section of our Web site:

Monomer Template (6.22 kb)
Alkaloid Template (31.9 kb)
Steroid Template (7.35 kb)
Terpene Template (12.4 kb)
Tipped Rings Template (1.83 kb)
Solid Phase Synthesis Resins (3.81 kb)
Template for Phosphorus Compounds (2.5 kb)
Template for Carbonyls (3.1 kb)
Newman Projections (6.6 kb)
Lewis Structures (12.2 kb)
Chem Quiz (4.3 kb)

7. Creating Special Graphical Objects

7.1 Objectives

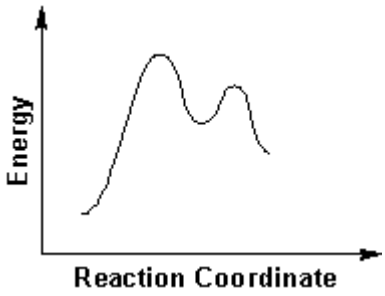
This chapter will familiarize you with the creation of graphical objects, so switch to the Draw mode before proceeding with any exercise in this chapter.

You will learn how to use Draw mode tools for creating the following objects:

- a diagram of the energy of reaction;
- various types of orbitals;
- vacuum distillation apparatus;
- a two-chain DNA strand;
- lipids and micelles; and
- multi-page layout posters.

7.2 Drawing the Energy of Reaction Diagram

This section is based on the movie **diagram.exe** which can be downloaded from our web site or found in the Movies folder.

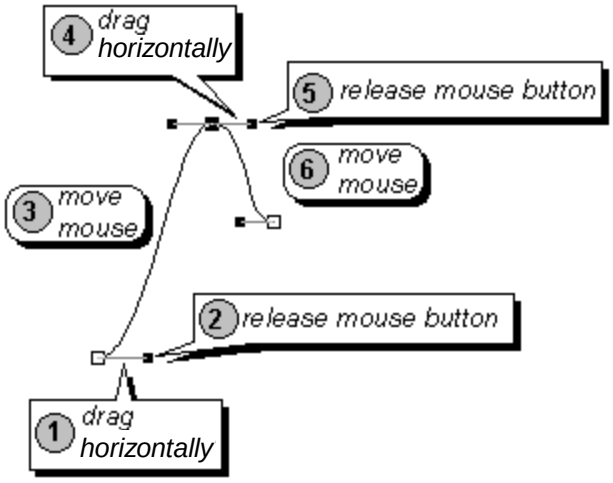


Switch to the mode and select the **Polyline** tool

7.2.1 Drawing a Curve

1. Drag horizontally to the right from the starting point of the curve to stretch the control line.
2. Release the mouse button.
3. Move the mouse up to draw the first segment of the curve.
4. Drag horizontally to the right to stretch the control lines. By changing the length of the control lines you can modify the form of the curve segment.
5. Release the mouse button.

6. Move the mouse down to draw the next segment.



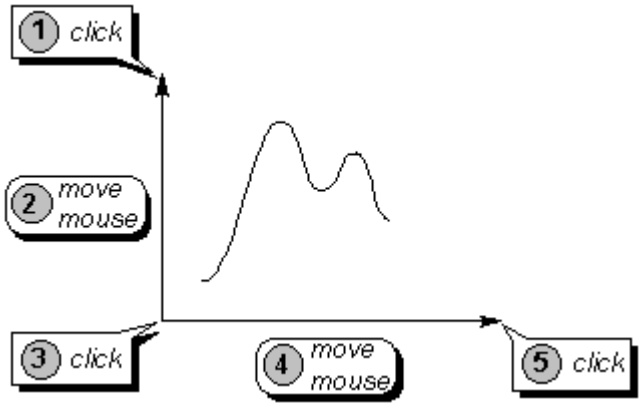
7. Repeat the above steps to draw the next two segments.
8. Click the right mouse button to finish drawing the curve.

7.2.2 Drawing the X and Y axes

Make sure that the Polyline tool is switched on.

Select the **Draw Arrow** tool . In the **Arrow** panel from the **Arrow Type** drop-down list choose the two way arrow .

1. Click at the endpoint of the Y axis.
2. Move the mouse down vertically to draw the axis.
3. Click to fix the point of the axes' intersection.
4. Move the mouse horizontally to the right to draw the X axis
5. Click to fix the endpoint of the X axis.



6. Click the right mouse button to finish drawing the axes.

> **Tip** You can easily draw the axes at a right angle by previously choosing the **Snap on Grid** and/or **Show Grid** command (**Options** menu).

7. Add inscriptions using the **Text** and **Rotate 90°** tools.

7.3 Drawing Different Kinds of Orbitals

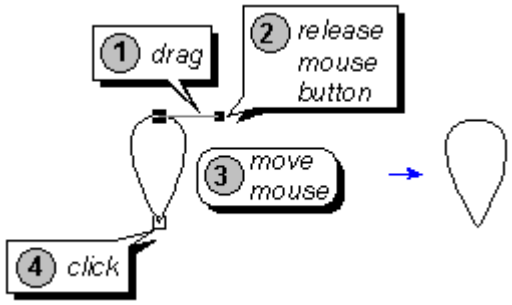
This section is based on the movie **orbital.exe** which can be downloaded from our web site or found in the Movies folder.

Switch to the Draw mode.

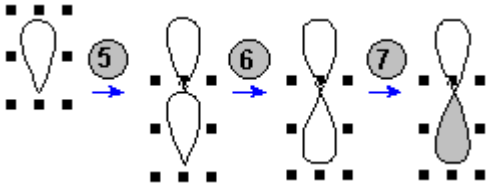
I. **To draw this orbital** **do the following**:

Select the **Polygon** tool .

1. Drag horizontally to the right from the starting point of the orbital to stretch the control line.
2. Release the mouse button.
3. Move the mouse down to draw the body of the orbital.
4. Click to fix the orbital.

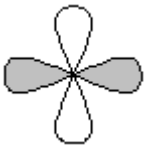


5. Right-click twice to finish drawing the orbital and to quickly switch to the **Select/Move/Re-size** tool . Position the cursor over the selected orbital; while holding down the CTRL key drag it down to make a copy of the drawn orbital.
6. Choose the **Flip Top to Bottom** button to flip the lower segment of the orbital. Align the segments by moving them.
7. Point to the gray color button in the **Color Palette** (at the bottom of the workspace) and click with the left mouse button to change the fill color of the orbital segment.



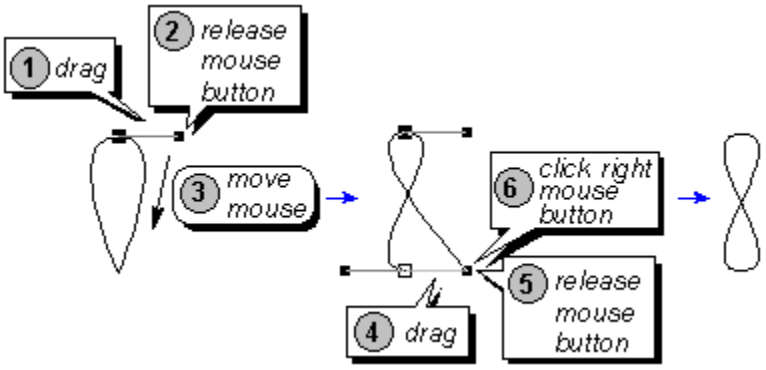
> **Tip** To quickly center the orbital segments, select them and click the **Center Horizontally** button .

8. Select both segments of the orbital and click the **Group** button . Now you can manipulate the segments as a single object, e.g. rotate using the **Select/Move/Rotate** tool .

II. **To draw the orbital**  **do the following**:

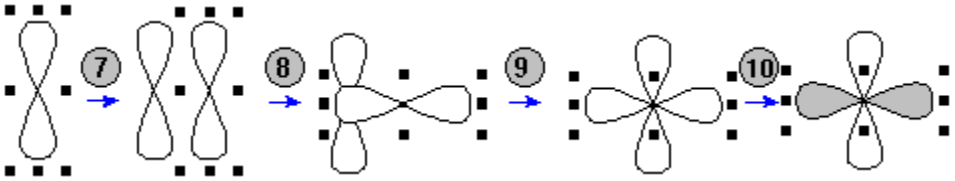
Select the **Polygon** tool .

1. Drag horizontally to the right from the starting point of the orbital to stretch the control line.
2. Release the mouse button.
3. Move the mouse down to draw the body of the orbital.
4. Drag horizontally to the right to stretch the control lines. Note that to make the two segments of the orbital identical, make the lengths of the control lines equal.
5. Release the mouse button.
6. Right-click to finish drawing the orbital and to switch to the **Select/Move/Re-size** tool .



> **Tip** You can draw the symmetrical orbital easier by previously choosing the **Snap on Grid** command (**Options** menu).

7. Select the orbital and holding down the CTRL key drag to make a copy of it.
8. Choose the **Rotate 90°** button .to rotate the copy of the orbital.
9. Move the copy by dragging it.
10. Point to the gray color button in the **Color Palette** and click with the left mouse button to change the color of the orbital:

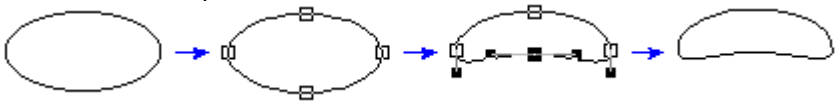


> **Tip** To quickly center the orbitals, select them and click the **Center Horizontally** button .

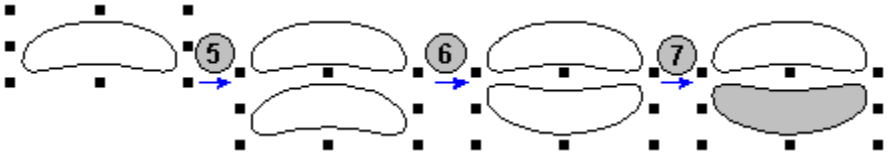
11. Select both orbitals and click the **Group** button . Now you can manipulate the orbitals as a single object, e.g. rotate using the **Select/Move/Rotate** tool .

III. **To draw this orbital** **do the following:**

1. Select the **Ellipse** tool and drag in the workspace to draw an ellipse.
2. From the **Objects** menu choose the **Convert to Polyline** command.
3. Select the **Edit Nodes** tool.
4. Drag the lowest node up.



5. Click the right mouse button to switch to the **Select/Move/Re-size** tool.
6. Select the orbital by clicking on its contour and holding down the CTRL key drag to make a copy of it.
7. Choose the **Flip Top to Bottom** button to flip the lower orbital.
8. Point to the gray color button in the **Color Palette** and click on the left mouse button to change the color of the orbital.

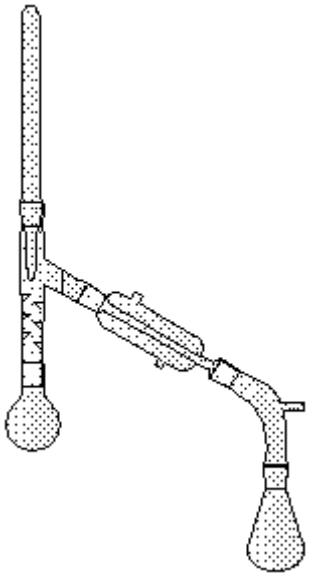


> **Tip** To quickly center the orbitals, select them and click the **Center Horizontally** button .

9. Select both orbitals and click the **Group** button. Now you can manipulate them as a single object.

7.4 Drawing Vacuum Distillation Apparatus

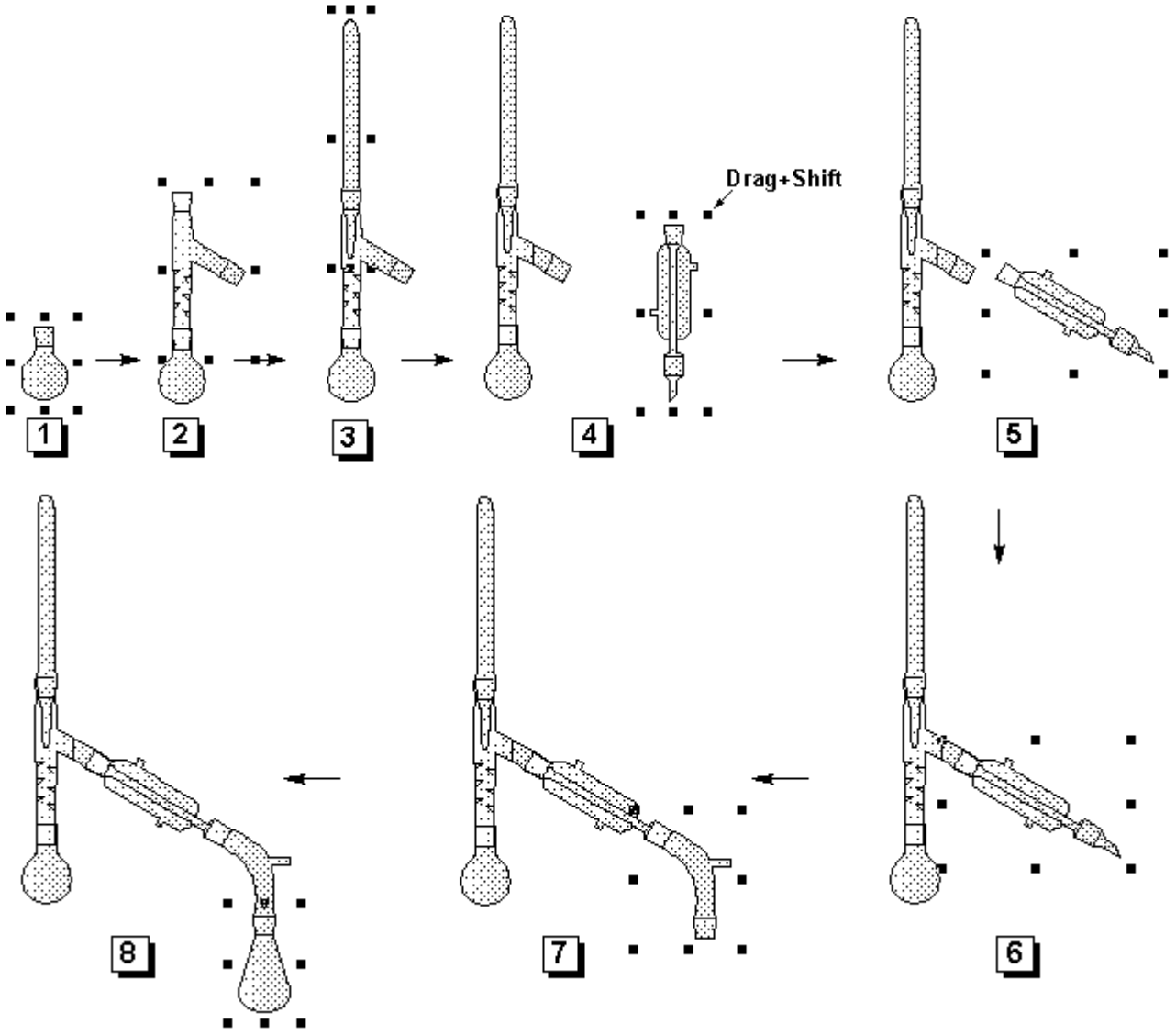
This section is based on the movie **apparat.exe** which can be downloaded from our web site or found in the Movies folder.



Switch to the **Draw** mode and set 50% zoom.

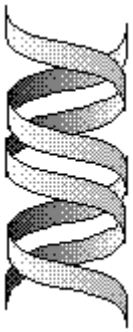
1. In the **Template Window** choose the **Lab Kit** tab from the **Template List**.
2. Select the **round-bottom flask** by clicking on it. Click on the workspace to place the selected template. Then right-click to hide the template shadow.
3. Open the **Template Window**. Select the **vigreux distillation column with connecting adapter.** Connect it to flask by clicking and right-click to hide the template shadow.
4. From the Template Window choose **thermometer** and connect it by clicking as shown. Hide the template shadow.
5. From the Template Window choose the **distillation column** and place it on the workspace near the apparatus by clicking. Right-click to hide the template shadow and switch to the **Select**/**Move**/**Re**-**size** tool .
6. Click on any selection handle (black squares surrounding the distillation column) to quickly switch to the **Select**/**Move**/**Rotate** tool .
7. Rotate the selected object 60° counter-clockwise by dragging any selection handle. The informative cursor will show you the angle of rotation (if the corresponding option has been selected in the **General** tab of the **Preferences** dialog box (**Options** menu)). Note, that holding down the SHIFT key while rotating will constrain the angle of rotation to 15° and will help you to rotate the object exactly by 60°.
8. Move the column by dragging to attach it to the apparatus.
9. From the **Template Window** select the **vacuum adapter** and attach it to apparatus.

10. Complete the drawing by connecting the **receiving flask**.



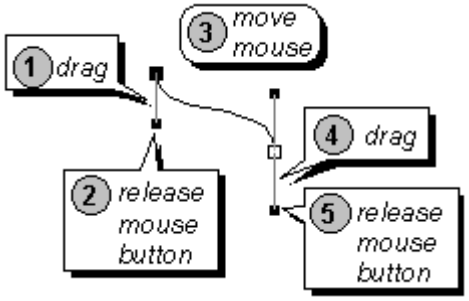
7.5 Drawing a Two-chain DNA Strand

This section is based on the movie **dna_ch.exe** which can be downloaded from our web site or found in the Movies folder.

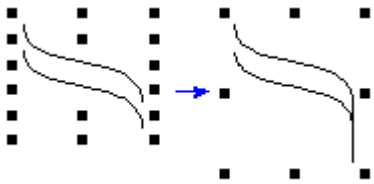


Switch to the Draw mode and select the **Polyline** tool.

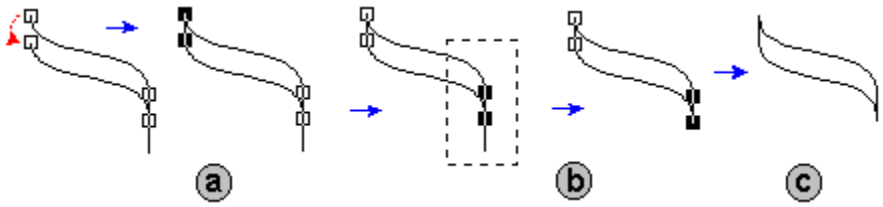
1. Drag vertically down from the starting point of the curve to stretch the control line;
2. Release the mouse button.
3. Move the mouse to the right to draw the curve.
4. Drag vertically down to stretch the control lines. By changing the length of the control lines you can modify the form of the curve.
5. Release the mouse button and right-click twice to finish drawing the curve and to switch to the **Select/Move/Re-size** tool.



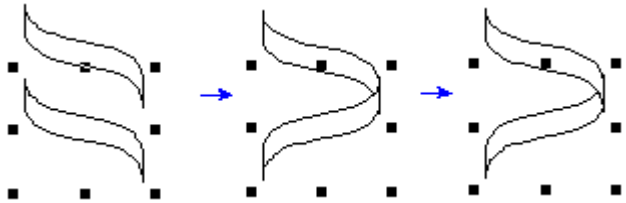
6. Place the mouse pointer over the selected curve and holding down CTRL+SHIFT keys drag it down (holding down the CTRL key while dragging leaves behind an instant copy of the object and holding down the SHIFT key forces the object to move strictly vertically or horizontally).
7. Select both curves by dragging the selection rectangle around them or by clicking on each of the curves while holding down the SHIFT key, then choose **Connect Lines** (in the **Object** menu) to connect the right ends of the curves.



8. Choose the **Edit Nodes** tool on the Editing toolbar (at the top of the workspace). Proceed with the following to draw a segment:
   a) Click the **Connect Vertices** button to connect the end nodes with a line.
   b) Select the right two nodes by dragging the selection rectangle around them and click the **Convert to Line** button.
   c) Click the right mouse button to leave the Edit Nodes mode and to switch to the **Select/Move/Re-size** tool.

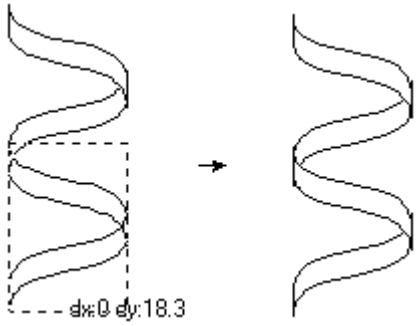


9. Make a copy of the obtained segment by dragging it with CTRL+SHIFT as described in step 2. Click the **Flip Left to Right** button to flip the segment and then click the **Send to Back** button to send the segment to the background.



> **Tip** It may take some time to correctly position the segments by manual moving them. To align their position automatically, select both segments and apply the **Center Horizontally** tool to the segments.

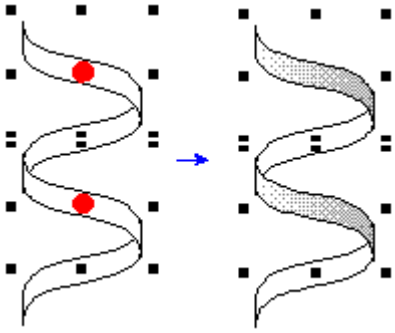
10. Select both segments by dragging or clicking while holding down the **Shift** key and make a copy of them (CTRL+drag). Correct the position using the directions in the previous step:



11. Select the segments marked with bullets in the picture below by clicking on them while holding down the SHIFT key. Double click on any of them to open the **Objects** panel. In the Fill tab specify the following settings:

    Style - ***Shade*** ;
    Color -white;
    Pattern- ;
    Shade - -30%

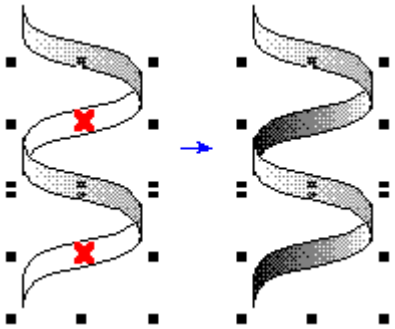
    and click **Apply**:



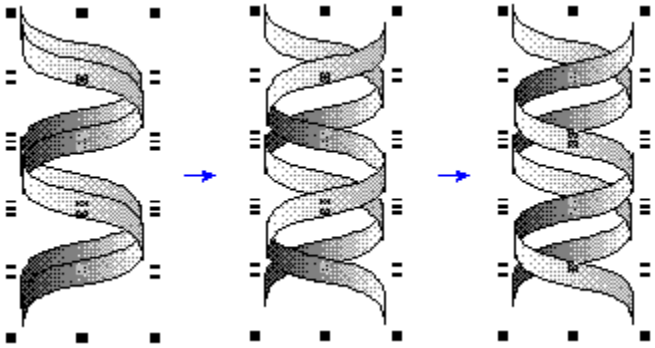
12. Select the other two segments (they are marked with crosses in the figure below) and specify the following settings in the Objects panel:

    Style - ***Shade*** ;
    Color -white;
    Pattern- ;
    Shade - -95%

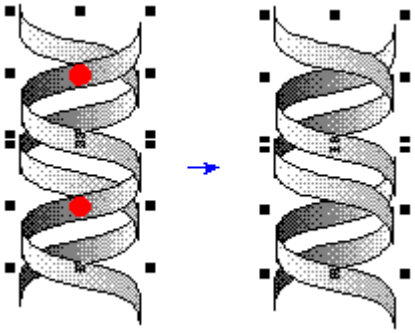
and click **Apply** to obtain the following spiral:



13. Select the whole spiral by dragging the selection rectangle so that it includes all the spiral segments and make a copy of it by dragging+CTRL. Click the **Flip Left to Right** and then **Flip Top to Bottom** buttons:



14. Select the segments marked with bullets in the picture below by clicking+SHIFT and click the **Send to Back** button .



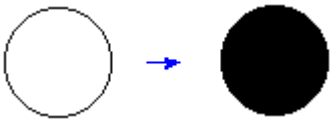
7.6 Drawing Lipids and Micelles

This section is based on the movie **lipid.exe** which can be downloaded from our web site or found in the Movies folder.

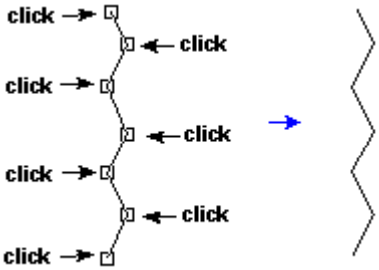
7.6.1 Drawing the lipid

Switch to the Draw mode.

1. Select the **Ellipse** tool. Drag in the workspace holding down the SHIFT key to draw a circle. Click with the left mouse button on the black color from the **Color Palette** (above the status bar) to color the fill of the circle.

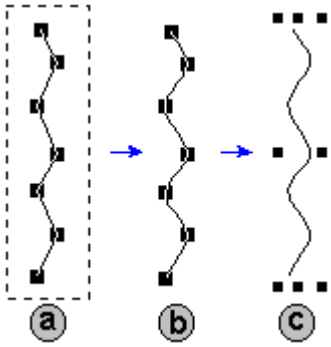


2. Choose the **Polyline** tool. Click repeatedly in the workspace near the circle to draw the carbonic tail and click the right mouse button to finish drawing.



> **Tip** To easily draw the symmetric zigzag line, you may previously choose the **Snap on Grid** and/or **Show Grid** command (**Options** menu).

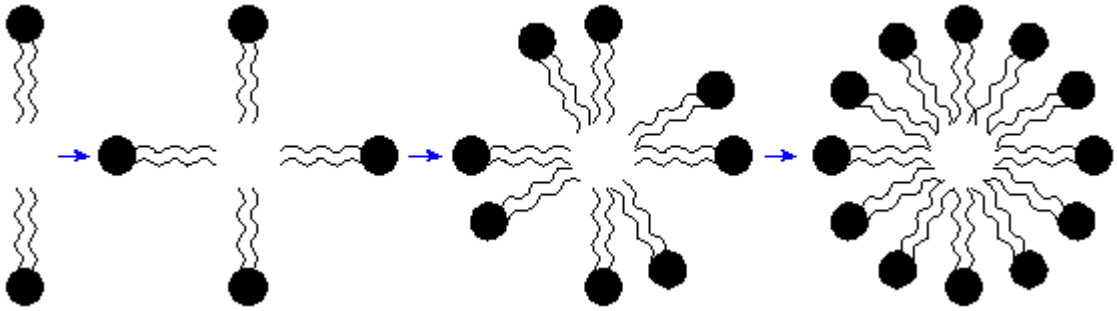
3. Choose the **Edit Nodes** tool and smooth the zigzag line in the following way:
   a) Select all the nodes of the drawn polyline by dragging the selection rectangle around it. Note that selected nodes become black.
   b) Click on the **Convert to Curve** button and then the **Smooth** button Smooth.
   c) Click the right mouse button to switch to the **Select**/**Move**/**Re**-**size** tool.



4. Position the mouse pointer over the curve and drag it holding down the CTRL key to leave the copy of the curve behind.
5. Arrange the tails as shown by dragging them.

Tip If you select all the elements of the phospholipid and click the **Group** button, you will be able to manipulate them as a single object, e.g. rotate it using the **Select**/**Move**/**Rotate** tool.

Try drawing the micelle picture using the copying feature (Ctrl + drag), Group, Rotate 90°, Select/Move/Rotate as well as the aligning and flipping tools :

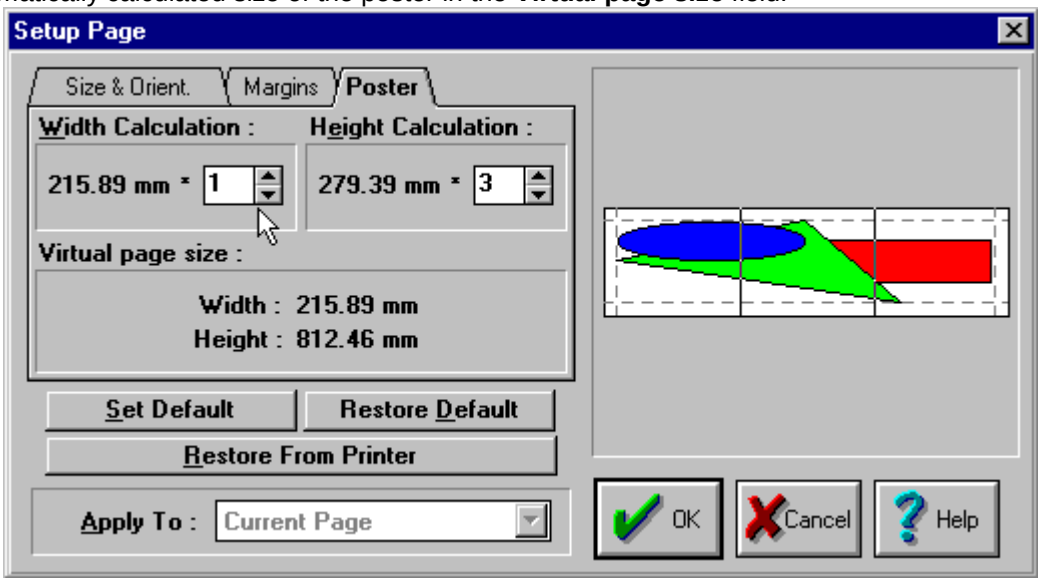


7.7 Creating a Poster

Using ChemSketch you can quickly draw a poster and print it on paper of any format. ACD/ChemSketch will automatically separate the poster into pages; the only thing you have to do (besides design them) is attach them.

This section is based on the movie **poster.exe** which can be downloaded from our web site or found in the Movies folder.

1. From the **File** menu choose the **Page Setup** command.
2. Select the **Poster** tab in the dialog box that appears. Set the number of standard pages you want your poster to consist of by clicking on the spin buttons. Note that you can see the automatically calculated size of the poster in the **Virtual page size** field:



3. In the **Size & Orient** and **Margins** tabs set the page margins and orientation.
4. Click

.
5. Draw your poster using the tools in the Structure and Draw modes. Note that you can use the **Paste** and **Paste Special** commands from the **Edit** menu to insert objects (text, pictures and etc.) created in other Windows applications . You can also edit these objects using OLE.
6. In the **Preferences** dialog box (**Options** menu) select the **View Printable area** check box in the **General** tab, if you want to see how your poster will be divided into individual pages while being printed.
7. Choose the **Printer Setup** command from the **File** menu.
8. In the **Select Printer** dialog box choose the **Set Up** button

and in the **Font** tab select the **Print TrueType as Graphics** option. Note that this step may be different for each printer.
9. Click **OK**.

10. Choose the **Print** command from the **File** menu or click the **Print** button on the General toolbar to print your poster.
11. Attach the pages.

8. Calculating Macroscopic Properties

8.1 Overview

ACD/ChemSketch is so versatile in its drawing capabilities that it is possible to overlook the unique macroscopic properties predictions which are built right into it. These include prediction of

- molecular weight;
- percentage composition;
- molar refractivity;
- molar volume;
- parachor;
- index of refraction;
- surface tension;
- density;
- dielectric constant; and
- polarizability.

In this Chapter, the simple means to calculate these properties is described. The algorithms for calculating these properties are briefly described, and a summary of the agreement is shown for calculated *vs*. experimental values for several hundred compounds.

Please note, that in this chapter, “properties” is used to mean physico-chemical values, in contrast to the general use of “properties” in ChemSketch documents, where the characteristics of the graphic display are referred to. For example, the **Structure Properties** command in the Tools menu permits you to set font size, bond thickness, color, *etc*.

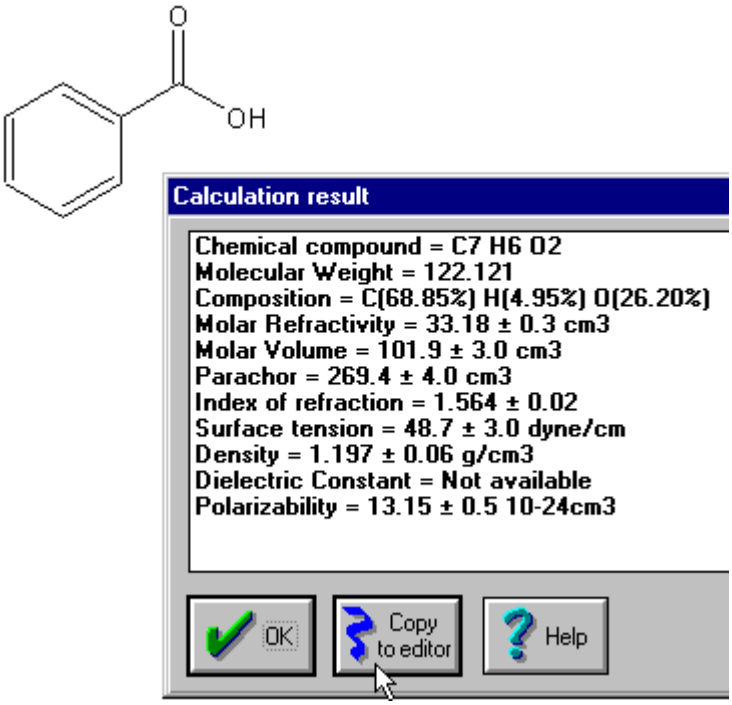
8.2 Calculating Macroscopic Properties

8.2.1 Menu Command

To determine any one or all of the following molecular properties, when in Structure mode, draw a structure, select **Tools** and then choose the **Calculate…** menu command. This permits calculation of

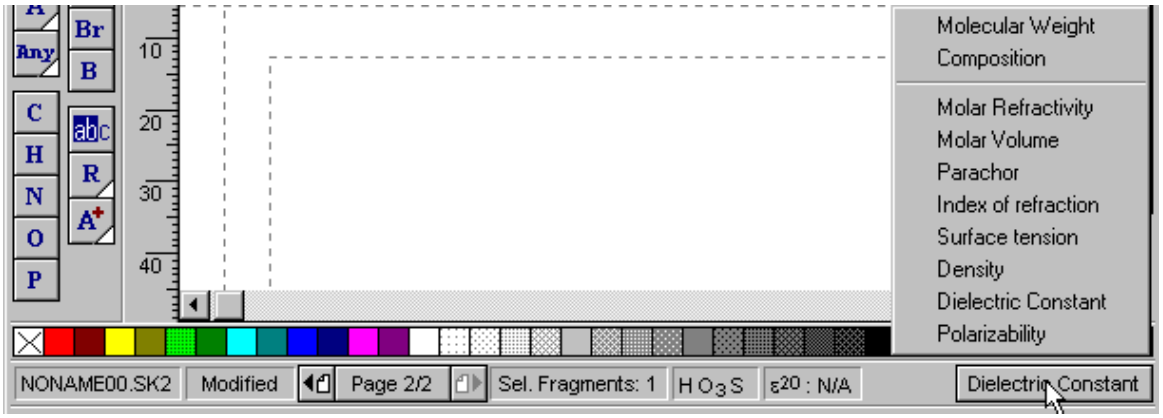
- molecular weight;
- percentage composition;
- molar refractivity;
- molar volume;
- parachor;
- index of refraction;
- surface tension;
- density;
- dielectric constant;
- polarizability; or
- all properties at once.

Once chosen, the calculated property is displayed in a **Calculation Result** dialog box. The text content of this can be immediately pasted on the ChemSketch screen if desired by clicking on the Copy to Editor button. For example, choosing **Tools>Calculate…>All properties** for benzoic acid will show the following dialog:



8.2.2 Automatic Display on Status Line

It is also possible to view the macroscopic property directly on the status line as shown:



Just click on the box to the far right on the status line and choose the property desired. By default, this is set to molecular weight. In the example shown, the dielectric constant, ε^{20}, has been specified.

8.3 Algorithms for Calculating Macroscopic Properties

At the heart of the additive-constitutive calculation algorithm of all physico-chemical properties in ChemSketch lies the presumption that these properties can be estimated using additive atomic or group increments. Apart from molecular weight (MW), which is trivial to calculate, the algorithms may be divided into three general groups:

- basic macroscopic properties: Molar Volume (MV), Molar Refractivity (MR) and Parachor (P_r);
- derived macroscopic properties: density (*d*) , refractive index (*n*) and surface tension (γ); and
- the dielectric constant ε (Permittivity).

Basic macroscopic properties such as Molar Volume (MV), Molar Refractivity (MR) and the Parachor (P_r) are calculated first for the input structure. The atomic additive increments in such an algorithm depend on the bonds (single, double, aromatic, *etc*.) of this atom and on neighboring atoms. ChemSketch rapidly analyzes the input structure to determine the class of each atom, *i.e.,* whether it is cyclic, aromatic, aliphatic, *etc*.

The prediction algorithms for density (*d*) , refractive index (*n*) and surface tension (γ) are founded on well known physico-chemical formula which can be found in most physical chemistry textbooks. These express *d, n* and γ as functions of MV, MR or P_r. Once the MV, MR or P_r, have been predicted by additive means, it is straightforward to predict *d*, *n* and γ using these formula.

The determination of the additive-constitutive atomic increments for MV, MR and P_r were obtained internally by ACD using large experimental data bases relating structure to density, refractive index and surface tension. The MV, MR and P_r were recalculated from *d*, *n* and γ. These parameters are proprietary information of Advanced Chemistry Development.

The prediction of the dielectric constant ε (permittivity) resembles very closely the prediction of Boiling Point, which is a separate ACD product from ChemSketch. Senior scientists at ACD discovered an additive function, which relates the dielectric constant to other macroscopic properties which can be additively treated, such as MV. Once this relationship was discovered, the additive-constitutive atomic increments for this function were obtained using large Data Bases consisting of molecular structures and their observed dielectric constants. Using the function and estimated MV for the input structure, its dielectric constant can be quickly predicted.

8.3.1 Molar Volume, MV

By definition,

$$MV = \frac{MW}{d}.$$

ChemSketch calculates molar volume from additive increments. The additive atomic increments were obtained using a Data Base of density and calculated MW.

8.3.2 Molar Refractivity, MR

The Lorentz-Lorenz equation relates refractive index, density, and refractive index:

$$MR = \frac{n^2 - 1}{n^2 + 2} \cdot \frac{MW}{d}$$

ChemSketch calculates molar refractivity from additive increments. The additive atomic increments were obtained using a Data Base of density, refractive index and calculated MW.

8.3.3 Parachor, P_r

By definition,

$$P_r = | \frac{MW}{d} | \gamma^{1/4}$$

ChemSketch calculates the parachor from additive increments. The additive atomic increments were obtained using a Data Base of density, surface tension, and calculated MW.

8.3.4 Density, *d*

By definition,

$$d = \frac{MW}{MV}$$

ChemSketch calculates the density from MW and the calculated molar volume (see above).

8.3.5 Refractive Index, *n*

By the Lorentz-Lorenz equation,

$$n = \sqrt{\frac{2 \cdot MR + MV}{MV - MR}}$$

ChemSketch calculates the refractive index from the molar volume and molar refractivity, both of which are calculated as above.

8.3.6 Surface Tension, γ

By definition,

$$\gamma = | \frac{P_r}{MV} |^4$$

ChemSketch calculates the surface tension from calculated MV (see above) and calculated P_r (see above).

8.3.7 Dielectric Constant, ε (Permittivity)

$$f(\varepsilon) = f(MV, AdditiveFunction)$$

ChemSketch calculates the dielectric constant from calculated MV (see above) and a proprietary empirical additive function.

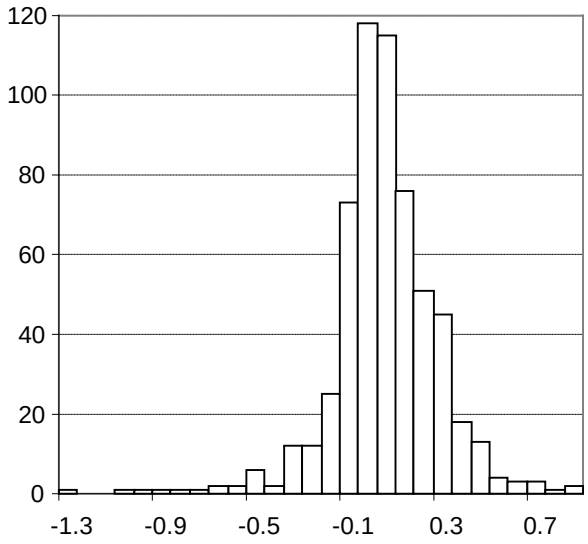
8.3.8 Polarizability

This property is calculated from the Molar Refractivity (MR) (see Section 8.3.2) as follows:

$$Polarizability = 0.3964308 \cdot MR$$

8.4 Correlation Statistics with Experimental Data

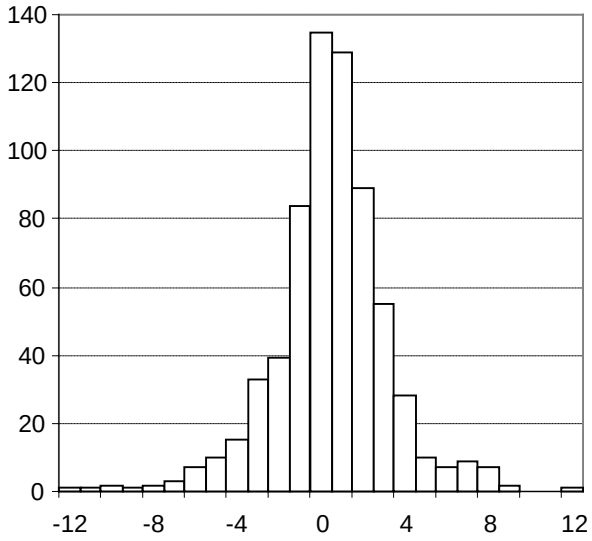
8.4.1 Distribution of Molar Refractivity Prediction Error



Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD Molar Refractivity Estimation Error
Number of tested structures:	592

$MR_{exp} = 0.99901(\pm 0.00067)\ MR_{calc} + 0.026(\pm 0.025)$ R=0.999867, StD=0.23

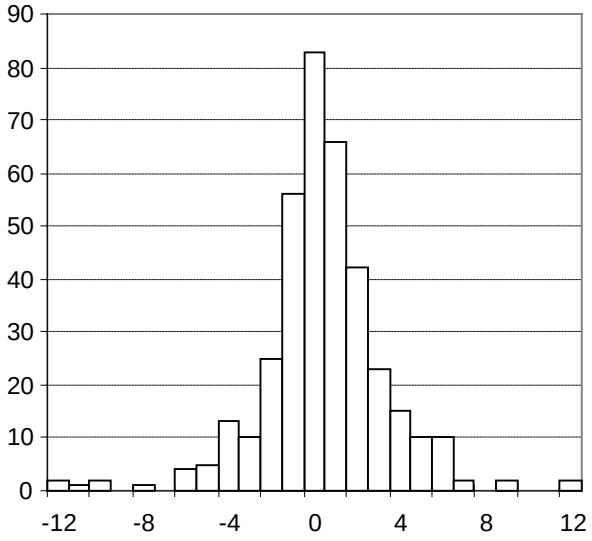
8.4.2 Distribution of Molar Volume Prediction Error



Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Molar Volume Estimation Error
Number of tested structures: 671

$MV_{exp} = 0.9989(\pm 0.0020)\ MV_{calc} + 0.18(\pm 0.29)$ R=0.998626, StD=2.74

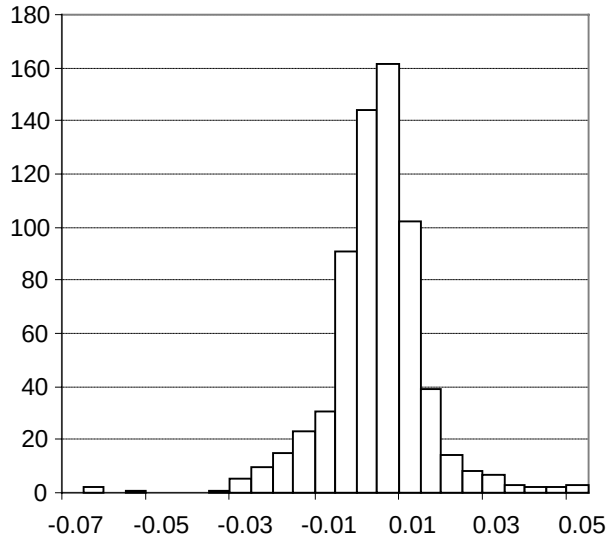
8.4.3 Distribution of the Parachor Prediction Error



Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Parachor Estimation Error
Number of tested structures: 377

$Pr_{exp} = 0.9978(\pm 0.0015)\ Pr_{calc} + 0.68(\pm 0.46)$ R=0.99958, StD=3.11

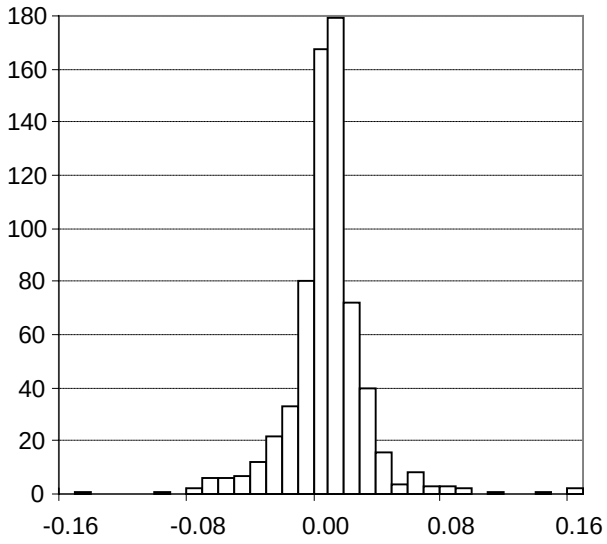
8.4.4 Distribution of the Refractive Index Prediction Error



Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Refractive Index Estimation Error
Number of tested structures: 665

$$n^{20}_{exp} = 0.98035(\pm 0.0073)\ n^{20}_{calc} + 0.028(\pm 0.011) \qquad R=0.982,\ StD=0.012$$

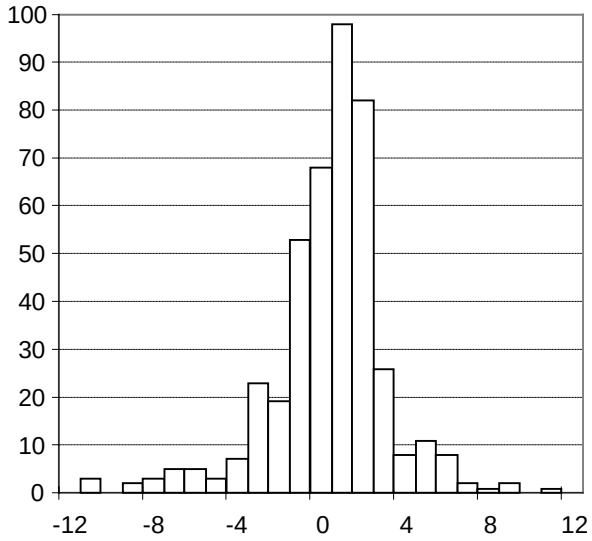
8.4.5 Distribution of the Density Prediction Error



Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Density Estimation Error
Number of tested structures: 671

$$d^{20}_{exp} = 0.9947(\pm 0.0036)\ d^{20}_{calc} + 0.0052(\pm 0.0036) \qquad R=0.995683,\ StD=0.028$$

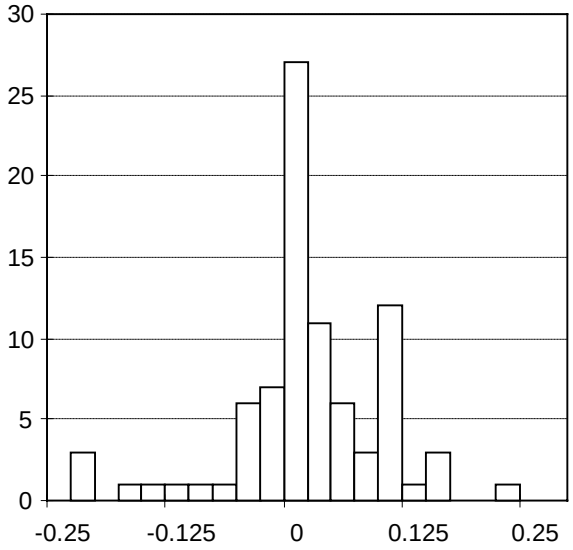
8.4.6 Distribution of the Surface Tension Prediction Error



Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Surface Tension Estimation Error
Number of tested structures: 432

$st^{20}_{exp} = 0.998(\pm 0.018)\ st^{20}_{calc} + 0.08(\pm 0.53)$ R=0.934720, StD=2.84

8.4.7 Distribution of the Dielectric Constant (Permittivity) Estimation Error



Vertical scale: Number of Tested Structures
Horizontal scale: Dielectric constant (Permittivity) Estimation Error
Number of tested structures: 85
*** Note *** Derived only for hydrocarbons

$\varepsilon_{exp} = 1.005(0.033)\varepsilon_{exp} - 0.013(0.072)$ R=0.9588, StD=0.079

9. Special Function Keys

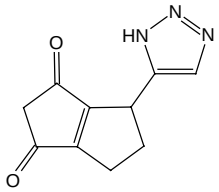
The ChemSketch Window is an extremely versatile molecular structure input editor. For this reason, several ACD software items are now accessible as single buttons from the ChemSketch interface. This Chapter describes two special add-on modules which can also be accessed from the ChemSketch interface. ACD/Tautomers is now included with both ACD/ChemSketch commercial and freeware; and ACD/Dictionary is available only with the ACD/ChemSketch commercial software.

9.1 Tautomers

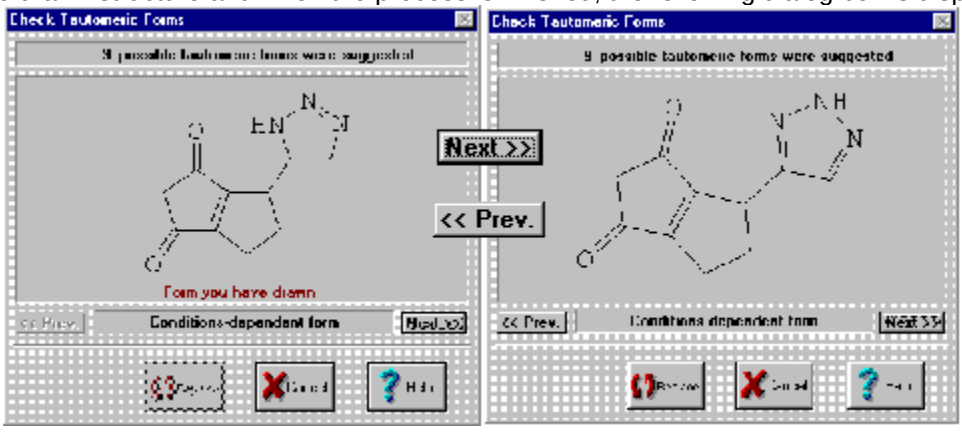
The Tautomers button will automatically check the structure that is drawn alone in the ChemSketch Window or which is selected from several other molecules and will automatically search for Tautomeric forms.

ACD/Tautomers is such a popular request item that we cover it here in some detail. For more information on Tautomers, as well as many examples of overlooked tautomers in the chemical literature, please refer to the **ACD/Tautomer User's Guide**.

1. Using the above technique draw the following structure:



2. Select the structure (use the **Select/Move** tool), click the **Check Tautomeric Forms** button on the Top toolbar. The program starts generating and checking tautomeric forms of the drawn structure and when the process is finished, the following dialog box is displayed:



3. To browse through all of the generated structures, click on the **Next >>** or **<< Prev.** buttons.

4. To replace the drawn structure with the currently displayed structure, click on the **Replace** button

.
5. Please refer to the **ACD/Tautomers User's** Guide for more information!

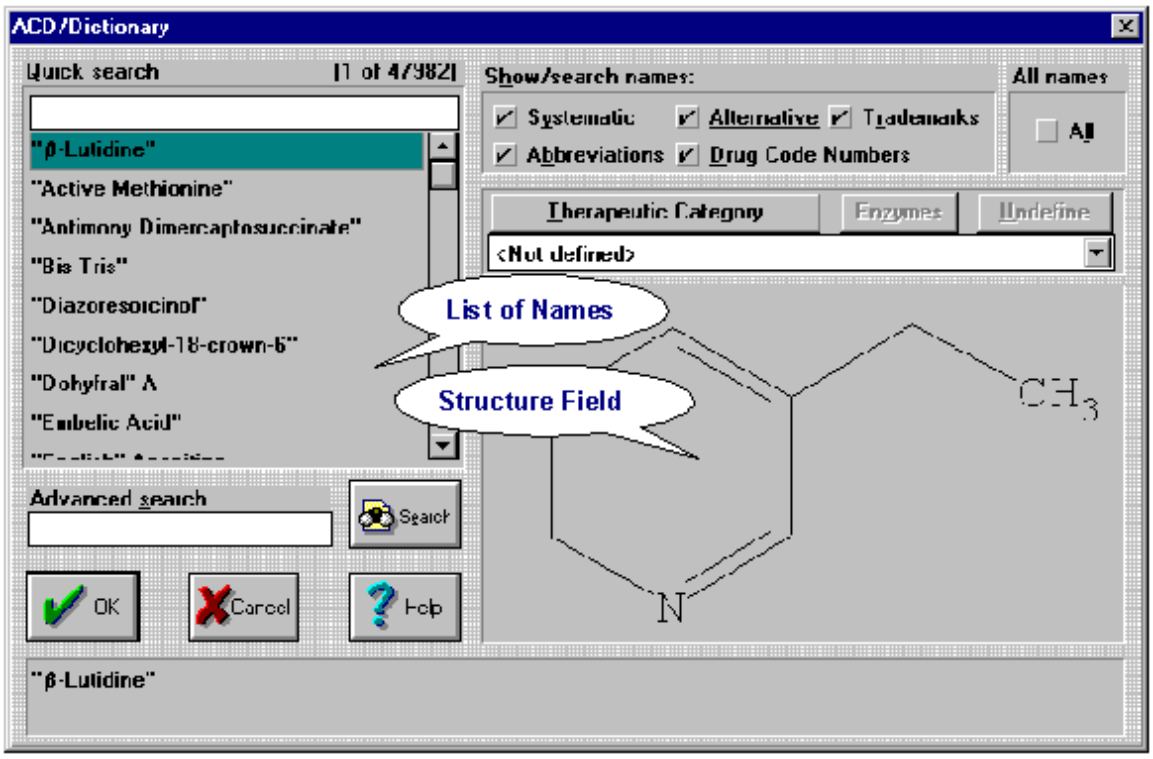
9.2 Dictionary

ACD/Dictionary is an add-in "Look-up" module, now included with all commercial copies of ACD/ChemSketch. It is extraordinarily useful at finding "chemicals" by their common names.

ACD/Dictionary finds chemical structures according to their chemical name. It contains almost 48,000 systematic and non-systematic names and their corresponding molecular structures. The dictionary is searchable by both the full chemical name and name fragments.

Although the many features of ACD/Dictionary are covered in the **ACD/Dictionary User's Guide**, we introduce it briefly here.

On the right **References** toolbar, click on the Dictionary button to view the **ACD/Dictionary** screen:



> **Note** If you purchased ACD/ChemSketch but do not see the ACD/Dictionary button in the ChemSketch Window when you are in Structure mode, please verify that you have correctly entered TWO registration numbers at the time of installation – one for **ACD/ChemSketch**, and one for the ACD/Dictionary add-in.

Please refer to the **ACD/Dictionary User's Guide** for more information!

10. Goodies

10.1 What are “Goodies”?

What are "goodies"? They are additional tool-buttons that extend the functionality of ChemSketch. They are, actually, implemented as ACD/ChemBasic programs associated with the 22 new ChemSketch buttons. ACD/ChemBasic is a special programming language that enables you to customize ACD software, and we think this is a great way to show off how useful it is—and at the same time make your ChemSketch even more versatile!

Note that you do not need to know anything about ACD/ChemBasic (although, if you wish, you can learn it by using the Goodies' code as example).

10.2 Where Can I Get Them?

These helpful buttons are already included in most ChemSketch 4.5 installations. To check if you already have them, look for all *.BAS files within your ChemSketch folder. If you don’t find any, you can download Goodies from our web site free of charge at

http://www.acdlabs.com/products/chem_dsn_lab/goodies.html

They are easy to install and to use. Just follow the installation instructions provided on the Web page and enjoy these new ChemSketch features.

Note that you can remove these new buttons from your ChemSketch toolbar at any time.

> **Note** ChemBasic Goodies buttons are only available when you are in Structure Mode.

10.3 Goodies

Below is the list of Goodies buttons that are available at the moment from our Web site:

Button	Function	How to use
Insert Page	Inserts blank pages at any place within your ChemSketch document. Note that the usual way - through a Pages/New menu - adds a page to the end of document.	∗ Go to the page before which you want to insert a blank page and click the Insert Page button.
Clone Page	Clones current page (together with its contents) a given number of times - it is very useful for filling in the document with page templates, tables, titles, etc. New pages are added at the end of a document.	∗ Make the page which you wish to clone active. ∗ Click the Clone Page button. ∗ In the dialog box that appears specify the number of clones and click OK.
Move/ Copy	Moves and copies pages - *i.e.*	∗ Go to the page which you wish to move or copy.

Button	Function	How to use
Page	changes page order in your document.	∗ Click the Move/Copy Page button. ∗ In the dialog box that appears type in number of the page after which you wish to place the current page and click **OK**. ∗ Select Yes in the Message Box which appears if you want to copy the current page. Select No if you want to just move it. Click Cancel to stop program execution.
Delete Pages	Deletes a range of pages at a time.	∗ Click the Delete Pages button. ∗ in the dialog box which appears type the sequence of pages to delete. ∗ You will be prompted about disabling Undo after program execution. Choose OK if you wish to delete the pages. Click Cancel to abort program execution.
Annotate Document	Annotates your documents based on the content of the leftmost top textbox on each page. This is very convenient for managing large documents and presentations.	∗ Open or create a document. ∗ Click the Annotate Document button. ∗ After program execution click on the page counter from the bottom status line to see page names.
Sketch-to-VRML Converter	Exports all the molecules in a current page into a VRML 2.0 file, which you may then view with Cosmo, GLView, or any other VRML browser.	∗ Draw structures which you wish to export in one page. ∗ Click the Sketch-To-VRML Converter button. ∗ Select **OK** in the Ready to export... message box which appears (or CANCEL to abort program). ∗ Type in the file name and path and click OK. Note that if you have typed in the filename only, the program will place the resulting WRL file in the same directory with sk2vrml.bas. ∗ Specify the desired structure presentation by typing the corresponding letter in the next dialog box and click OK.
SDF-to-Sketch Converter	Imports the data (molecules, texts, etc.) from a file in MDL's SDF format into ChemSketch document. Each record in the SDF file becomes a page. LIMITATION: no more than 100 records may be imported (ChemSketch document may contain 100 pages maximum). If the SDF file contains more than 100 records then you will be prompted about partial SDF conversion (and the number of successfully imported records).	∗ Click the SDF-To-Sketch Converter button. ∗ In the dialog box type in the full path and name (or mask - "*" and "?" are acceptable in the file-mask) of the SDF file which you want to import and click OK. If you type in the filename without specifying the full path, the program will search your SDF file in ChemBasic program directory. So, if you place the needed SDF file in the same directory with sdf2sk.bas then simply specify the file name without a path. If you place the SDF file in ChemBasic's program sub-directory then iyou need only type in the sub-directory name. ∗ If searching the result contains more than 1 file, the program will suggest you select one, then will ask for the field name. Specify the field name and click **OK**.
Document Browser	Looks through the directories to find specified ChemSketch documents as well as to search ChemSketch documents for the text string without opening them.	∗ Click this button and follow the instructions that appear in the messages. This is a very useful tool for searching and previewing ChemSketch documents
Table Wizard	Creates tables or/and aligns objects according to a specified number of rows and columns	To create a table and place the drawn objects into it ∗ Click the Table Wizard button. ∗ You will be informed about the number of objects on the page and some suggestions on how to align them. Select YES. ∗ Specify the number of rows and columns in the table. ∗ Then choose whether to create borders in the table.

Button	Function	How to use
		To create an empty table ∗ Run the Table Wizard with the blank page active. ∗ or ∗ Select NO in the message box that suggests that you should align objects.
Replace Element	Replaces all the atoms of a given type with atoms of another type in a chemical structure. This is very useful for drawing, for example, perfluorinated structures.	Note that program execution is possible only with a single structure on the page. ∗ Draw or leave only one structure on the page and click this button. ∗ In the dialog box that appears specify the element which you want to be replaced and click OK. ∗ In the next dialog box specify an element that should replace the one specified before and click **OK**.
Solution Calculator	Calculates the weight of a compound required for preparing a solution of the user-defined volume and molar concentration.	Note that program execution is possible only with a single structure on the page. ∗ Draw or leave one structure on the page and click this button. ∗ Specify the required molar concentration and solution volume in the dialog box. ∗ See the result in the Message Box that appears.
Label Printer	Quickly creates labels for chemicals and print them on the Avery Standard (45 template sheets included) or your own sheets	∗ Draw structures for which you want to create labels and click this button. ∗ You can create labels for structures from the *.sdf file if you run this program with an empty active page. ∗ For more information see lprinter.txt provided in the Goodies directory.
Peptide Builder	Builds a 3D peptide structure from the amino acids sequence.	∗ Refer to the pepbuild.sk2 provided in the Goodies directory as a guide to using this button.
Carbo-hydrate Builder	Builds a structure from carbohydrate abbreviated names.	∗ For information about how to work with this button refer to the sugarsk.txt file that you can find in the Goodies directory.
Reorder Pages	Allows you to cut-and-paste or copy-and-paste a sequence of pages to a new position within the same document.	∗ Open the document within which you want to reorder the pages. ∗ Click this button and follow the instructions in the messages.
Rename Pages	Changes the name of pages	∗ Open the document. ∗ Click this button. ∗ Type in the number of a page you want to name and click OK. ∗ Type the name and click OK. ∗ The names of the pages are shown when you click on the “Page 1/1” button at the bottom of your ChemSketch Window.
Insert Page Numbers/ Annotations	Inserts page numbers or complex annotations in your document. Note that annotation will be inserted in a left-bottom corner of the page.	∗ Open or create a document. ∗ Click the Annotate Pages button ∗ Type in a page annotation template in dialog box that appears and click OK. Annotation template keys: ∗ **$P** - inserts page numbers

Button	Function	How to use
		∗ **$N** - inserts pages names (that can be inserted using **Rename Pages** goody or using Pages/Rename command) You can also include any fixed text into your annotation template. *For example:* Template "**$P**" will insert page numbers Template "**$N**" will place page names in a left-bottom corner of each page Template "**Page $P**" will insert "Page 1", "Page 2", *etc.* annotations Template: "**Page $P: $N**" will insert "Page 1: Page Name", *etc.* Annotations Template that does not contain any keys will insert fixed text for each page - you can, for example, sign all pages with your name.
Create HTML	Exports all the selected pages of a current document into an HTML file, which you may then view with your favorite web-browser. **Note: Requires ChemSketch 4.01.**	∗ All the details may be found in FillTmpHelp.doc provided in the Goodies directory.
Sketch-To-SDF Converter	Exports all the structures from the current page or from the whole document into an SDF file.	∗ Open the page with the structures you want to export. ∗ Choose this button and choose what you want to import - the current page or the whole document. Click OK. ∗ Specify the name and the path for an *.sdf file. Note that if you type in the filename only, the program will place the resulting sdf file in the same directory with expsdf.bas file.
Explicit Hydrogens	Explicitly shows hydrogens in the drawn structure(s).	∗ * Draw structure(s) on the page and click this button. **Note:** you can use standard ChemSketch command - Tools/Remove Explicit Hydrogens - to revert this goody action.
Remove Spectator Ions (Desalt)	An SDF file that contains one or more salt structure entries can be changed to a "one-molecule-per-entry" SDF file. This button removes the smallest ion, either by MW or by number of atoms. For example, sodium acetate will have the sodium atom removed, and acetic acid will remain behind. (Note: the molecule left behind is put into neutral form.)	∗ Specify the name and the path for an *.sdf file. Note that if you type in the filename only, the program will look for file in the Goodies directory. ∗ Then define a criterion for smallest part: mass or atom. ∗ The resultant SDF file will be saved in the same directory with the one you have specified under the newfile.sdf name. A special sample file, "salts.sdf" with 5 salts in it is placed in the Goodies directory for testing. Hint: use the "Import SDF" Goody to double-check Newfile.sdf.
Nucleic Acid Builder	Builds a 3D nucleic acid (DNA, RNA) structure (one or two chains) from your input sequence.	∗ Click this button and follow the instructions from the messages.